

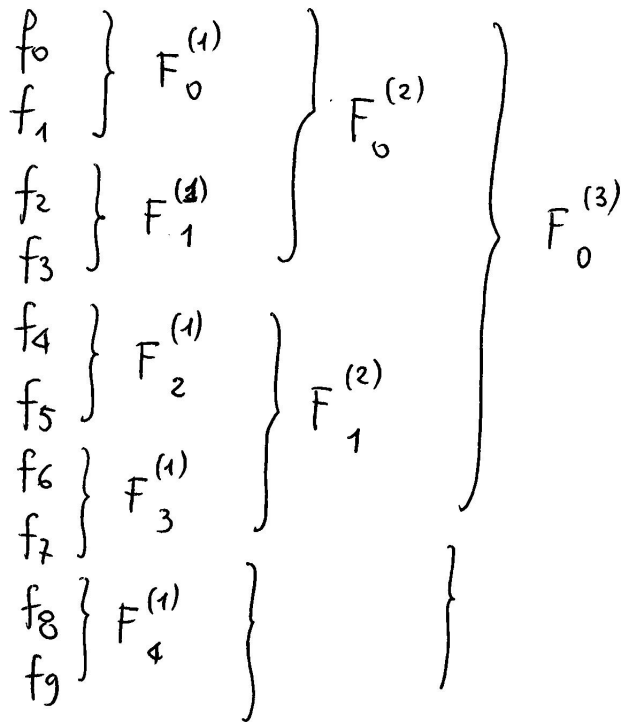
THE BLOCKING METHOD

①

The blocking method is based on the idea of

RECURSIVE BINNING

RUN: $X_0, X_1, X_2, \dots, X_{N-1}$ N data
 $f_0, f_1, f_2, \dots, f_{N-1}$ $f_i = f(X_i)$



$$F_0^{(1)} = \frac{1}{2} (f_0 + f_1)$$

$$F_1^{(1)} = \frac{1}{2} (f_2 + f_3)$$

⋮

$$F_0^{(2)} = \frac{1}{2} (F_0^{(1)} + F_1^{(1)})$$

$$= \frac{1}{4} (f_0 + f_1 + f_2 + f_3)$$

$$F_1^{(2)} = \frac{1}{2} (F_2^{(1)} + F_3^{(1)})$$

$$= \frac{1}{4} (f_4 + f_5 + f_6 + f_7)$$

⋮

$$F_0^{(3)} = \frac{1}{2} (F_0^{(2)} + F_1^{(2)}) =$$

$$= \frac{1}{8} (f_0 + f_1 + \dots + f_7)$$

Thus from the original data we generate

$F_0^{(1)} \dots F_{N/2}^{(1)}$ $N/2$ data

$F_0^{(2)} \dots F_{N/4}^{(2)}$ $N/4$ data

and so on

Now we want to compute the variance of the $F_i^{(k)}$ ②

But before, note that, IN EQUILIBRIUM (the distribution of X_i is always π , independent of time)

$$\langle f(X_i) \rangle_{MC} = \langle f \rangle_{\pi}$$

$$\langle F_i^{(1)} \rangle_{MC} = \langle \frac{1}{2} (f_{2i} + f_{2i+1}) \rangle_{MC} =$$

$$= \left(\langle f_{2i} \rangle_{MC} + \langle f_{2i+1} \rangle_{MC} \right) \frac{1}{2} = \langle f \rangle_{\pi}$$

$$\langle F_i^{(2)} \rangle_{MC} = \langle \frac{1}{2} (F_{2i}^{(1)} + F_{2i+1}^{(1)}) \rangle_{MC} = \langle f \rangle_{\pi}$$

All variables have the same average $\langle f \rangle_{\pi} = F$

Now, let us compute the variance

We begin with $\langle (F_i^{(1)} - F)(F_i^{(1)} - F) \rangle_{MC} = \Delta^{(1)}$

IN EQUILIBRIUM it DOES NOT DEPEND ON TIME.

We set $i=0$

$$\Delta^{(1)} = \langle \left(\frac{1}{2} f_0 + \frac{1}{2} f_1 - F \right)^2 \rangle_{MC} = \frac{1}{4} \langle (f_0 - F + f_1 - F)^2 \rangle_{MC}$$

$$= \frac{1}{4} \left[\langle (f_0 - F)^2 \rangle_{MC} + 2 \langle (f_0 - F)(f_1 - F) \rangle_{MC} + \langle (f_1 - F)^2 \rangle_{MC} \right]$$

$$= \frac{1}{4} \left[C(0) + 2C(1) + C(0) \right] = \frac{1}{2} \left[C(0) + C(1) \right]$$

$C(n)$ is the autocorrelation function

Now we compute

(3)

$$\begin{aligned}\Delta^{(2)} &= \left\langle \left(\frac{1}{4}f_0 + \frac{1}{4}f_1 + \frac{1}{4}f_2 + \frac{1}{4}f_3 - F \right)^2 \right\rangle_{MC} \\ &= \frac{1}{16} \left[\left\langle \left[(f_0 - F) + (f_1 - F) + (f_2 - F) + (f_3 - F) \right]^2 \right\rangle_{MC} \right] \\ &= \frac{1}{16} \left[\left\langle (f_0 - F)^2 \right\rangle_{MC} + \left\langle (f_1 - F)^2 \right\rangle_{MC} + \left\langle (f_2 - F)^2 \right\rangle_{MC} + \left\langle (f_3 - F)^2 \right\rangle_{MC} \right. \\ &\quad + 2 \left\langle (f_0 - F)(f_1 - F) \right\rangle_{MC} + 2 \left\langle (f_1 - F)(f_2 - F) \right\rangle_{MC} + 2 \left\langle (f_2 - F)(f_3 - F) \right\rangle_{MC} \\ &\quad + 2 \left\langle (f_0 - F)(f_2 - F) \right\rangle_{MC} + 2 \left\langle (f_1 - F)(f_3 - F) \right\rangle_{MC} \\ &\quad \left. + 2 \left\langle (f_0 - F)(f_3 - F) \right\rangle_{MC} \right] \\ &= \frac{1}{16} \left[4C(0) + 2 \cdot 3C(1) + 2 \cdot 2C(2) + 2C(3) \right] \\ &= \frac{1}{4} \left[C(0) + \frac{3}{2}C(1) + \frac{2}{2}C(2) + \frac{1}{2}C(3) \right]\end{aligned}$$

We can generalize the result

$$\begin{aligned}\Delta^{(3)} &= \frac{1}{2^3} \left[C(0) + \frac{7}{4}C(1) + \frac{6}{4}C(2) + \frac{5}{4}C(3) + \frac{4}{4}C(4) + \frac{3}{4}C(5) \right. \\ &\quad \left. + \frac{2}{4}C(6) + \frac{1}{4}C(7) \right]\end{aligned}$$

$$\begin{aligned}\Delta^{(k)} &= \frac{1}{2^k} \left[C(0) + \sum_{n=1}^{2^k-1} \frac{(2^k-n)}{2^{k-1}} C(n) \right] \\ &= \frac{1}{2^k} \left[C(0) + 2 \sum_{n=1}^{2^k-1} C(n) - \frac{1}{2^{k-1}} \sum_{n=1}^{2^k-1} n C(n) \right]\end{aligned}$$

Now let us define the "errors" σ_k^2 that are obtained by assuming that the variables $F^{(k)}$ are independent (uncorrelated)

$$\sigma_1^2 = \frac{1}{N/2} \text{Var } F^{(1)} = \frac{2}{N} \Delta^{(1)} = \frac{1}{N} [C(0) + C(1)]$$

of measures $F^{(1)}$

$$\sigma_2^2 = \frac{1}{N/4} \text{Var } F^{(2)} = \frac{4}{N} \Delta^{(2)} = \frac{1}{N} \left[C(0) + \frac{3}{2} C(1) + \frac{2}{2} C(2) + \frac{C(3)}{2} \right]$$

$$\sigma_3^2 = \frac{1}{N/8} \Delta^{(3)} = \frac{1}{N} \left[C(0) + \frac{7}{4} C(1) + \frac{6}{4} C(2) + \frac{5}{4} C(3) + \frac{4}{4} C(4) \right. \\ \left. + \frac{3}{4} C(5) + \frac{2}{4} C(6) + \frac{1}{4} C(7) \right]$$

$$\sigma_k^2 = \frac{1}{N/2^k} \Delta^{(k)} = \frac{1}{N} \left[C(0) + 2 \sum_{n=1}^{2^k-1} C(n) - \frac{1}{2^{k-1}} \sum_{n=1}^{2^k-1} n C(n) \right]$$

$$= \frac{1}{N} \left[C(0) + 2 \sum_{n=1}^{\infty} C(n) - 2 \sum_{n=2^k}^{\infty} C(n) - \frac{1}{2^{k-1}} \sum_{n=1}^{2^k-1} n C(n) \right]$$

goes to zero for $k \rightarrow \infty$

$$\approx \frac{1}{N} \left[C(0) + 2 \sum_{n=1}^{\infty} C(n) \right] = \text{correct error for the sample mean of } f: \bar{f}.$$

$$\sigma_k^2 - \sigma^2 \sim O\left(\frac{1}{m}\right) \quad [\text{Decreases slowly}]$$

↑
length of the block ($m=2^k$)

CONCLUSION:

The quantity σ_k^2 (the error on the $F^{(k)}$ assuming that these variables are UNCORRELATED) converges to the correct error σ^2 of the variables f_i

THE PRACTICAL PROCEDURE

• Compute $F_i^{(1)}$ $i: 0, \dots, \frac{N}{2} - 1$

$$\text{and } \sigma_1^2 = \frac{1}{N/2} \text{Var } F^{(1)} = \frac{2}{N} \left[\frac{1}{N/2} \sum_{i=0}^{N/2-1} (F_i^{(1)})^2 - \left(\frac{1}{N/2} \sum_{i=0}^{N/2-1} F_i^{(1)} \right)^2 \right]$$

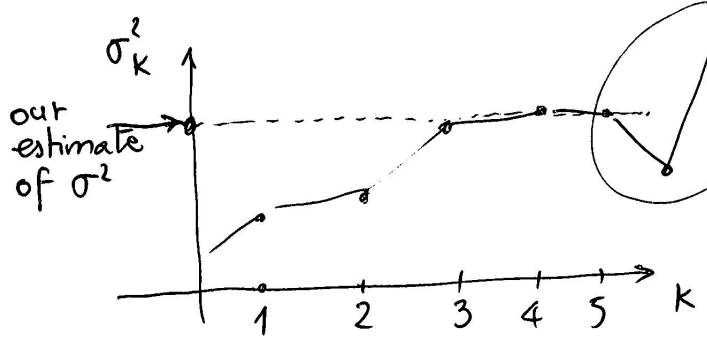
This is the variance estimator

• Compute $F_i^{(2)}$ $i: 0, \dots, \frac{N}{4} - 1 = m$

$$\sigma_2^2 = \frac{1}{m} \text{Var } F^{(2)} = \frac{1}{m} \left[\frac{1}{m} \sum_{i=0}^{m-1} (F_i^{(2)})^2 - \left(\frac{1}{m} \sum_{i=0}^{m-1} F_i^{(2)} \right)^2 \right]$$

and so on

• Plot σ_i vs. i (the level of blocking)



Fluctuations that cannot be correct (MC fluctuations)

We must have $\sigma_{k+1}^2 > \sigma_k^2$

The estimates increase with k