

## JACKKNIFE METHOD

①

Suppose we wish to compute  $\langle f \rangle_\pi$  and  $J(\langle f \rangle_\pi)$

Generate  $N$  number with probability  $\pi(x)$

$$X_1, \dots, X_N$$

Define the Jackknife averages

$$\bar{f}_i = \frac{1}{N-1} \sum_{\substack{j=1 \\ j \neq i}}^N f(X_j) \quad J_i = J(\bar{f}_i)$$

$\bar{f}_i$  is the sample mean in which we consider all data, except  $X_i$

Example  $N=4$

We compute

$$\bar{f}_1 = \frac{1}{3} (f(X_2) + f(X_3) + f(X_4)) \quad J_1 = J(\bar{f}_1)$$

$$\bar{f}_2 = \frac{1}{3} (f(X_1) + f(X_3) + f(X_4)) \quad J_2 = J(\bar{f}_2)$$

$$\bar{f}_3 = \frac{1}{3} (f(X_1) + f(X_2) + f(X_4)) \quad J_3 = J(\bar{f}_3)$$

$$\bar{f}_4 = \frac{1}{3} (f(X_1) + f(X_2) + f(X_3)) \quad J_4 = J(\bar{f}_4)$$

Note

$$\begin{aligned} \frac{1}{4} \sum_{i=1}^4 \bar{f}_i &= \frac{1}{3} \cdot \frac{1}{4} (3f(X_1) + 3f(X_2) + 3f(X_3) + 3f(X_4)) \\ &= \frac{1}{4} (f(X_1) + f(X_2) + f(X_3) + f(X_4)) \\ &= \bar{f} \end{aligned}$$

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This result is true in general

(2)

$$\begin{aligned}\mu_{JK} &= \frac{1}{N} \sum_i \bar{f}_i = \frac{1}{N} \sum_i \left[ \frac{1}{N-1} \sum_{\substack{j=1 \\ j \neq i}}^N f(x_j) \right] \\ &= \frac{1}{N(N-1)} \sum_{z=1}^N \left( \sum_{\substack{j=1 \\ j \neq i}}^N f(x_j) - f(x_i) \right) \\ &\quad \text{[we add } f(x_i) \text{ to the sum]} \\ &= \frac{1}{N(N-1)} \sum_{z=1}^N \left[ N\bar{f} - f(x_i) \right] \\ &= \frac{1}{N(N-1)} \left( \sum_{z=1}^N N\bar{f} - \sum_{z=1}^N f(x_i) \right) \\ &= \frac{1}{N(N-1)} \left( N^2\bar{f} - N\bar{f} \right) = \bar{f}\end{aligned}$$

For the sample mean the average of the jackknife averages is equivalent to  $\bar{f}$ .

$$\sigma_{JK}^2 = \frac{1}{N} \sum_i \bar{f}_i^2 - \mu_{JK}^2 \quad (\text{jackknife variance})$$

Now

$$\begin{aligned}\frac{1}{N} \sum_{z=1}^N \bar{f}_i^2 &= \frac{1}{N} \sum_{z=1}^N \left( \frac{1}{N-1} \sum_{\substack{j=1 \\ j \neq i}}^N f(x_j) \right)^2 \\ &= \frac{1}{N(N-1)^2} \sum_{z=1}^N \left( \sum_{j=1}^N f(x_j) - f(x_i) \right)^2 \\ &= \frac{1}{N(N-1)^2} \sum_{z=1}^N \left( N\bar{f} - f(x_i) \right)^2\end{aligned}$$

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$$\begin{aligned}
&= \frac{1}{N(N-1)^2} \sum_{i=1}^N (N^2 \bar{f}^2 - 2N\bar{f} f(x_i) + f(x_i)^2) \quad (3) \\
&= \frac{1}{N(N-1)^2} \left[ N^2 \bar{f}^2 \underbrace{\sum_{i=1}^N 1}_N - 2N\bar{f} \underbrace{\sum_{i=1}^N f(x_i)}_{N\bar{f}} + \underbrace{\sum_{i=1}^N f(x_i)^2}_{N\bar{f}^2} \right] \\
&= \frac{1}{(N-1)^2} \bar{f}^2 + \frac{N(N-2)}{(N-1)^2} \bar{f}^2
\end{aligned}$$

We plug in the result in  $\sigma_{JK}^2$  ( $\mu_{JK} = \bar{f}$ )

$$\begin{aligned}
\sigma^2 &= \frac{1}{(N-1)^2} \bar{f}^2 + \frac{N(N-2)}{(N-1)^2} \bar{f}^2 - \bar{f}^2 = \quad \text{Correction: here } \sigma^2 \text{ is } \sigma_{JK}^2 \\
&= \frac{1}{(N-1)^2} (\bar{f}^2 - \bar{f}^2)
\end{aligned}$$

Now note that the error  $\sigma$  on  $\bar{f}$  is

$$\sigma^2 = \frac{1}{(N-1)} (\bar{f}^2 - \bar{f}^2) \rightarrow \sigma^2 = (N-1) \sigma_{JK}^2$$

Thus, we can estimate

$$\sigma = \sqrt{(N-1) \sigma_{JK}^2}$$

- To compute the error on  $\bar{f}$  there is NO ADVANTAGE in using the Jackknife method
  - Results are equivalent
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④

The jackknife method is useful for estimating  
 $J(\langle f \rangle_{\pi})$

### AVERAGE

jackknife estimate

$$\text{est}[J(\langle f \rangle_{\pi})] = NJ(\bar{f}) - \frac{(N-1)}{N} \sum_{z=1}^N J(\bar{f}_i)$$

### ERROR

$$\sigma^2 = (N-1) \left[ \frac{1}{N} \sum_{z=1}^N J(\bar{f}_i)^2 - \left( \frac{1}{N} \sum_{z=1}^N J(\bar{f}_i) \right)^2 \right]$$

**CORRECTION:**  
Add a bar on top  
of the last term.  
The error depends  
on  $J_i = J(\bar{f}_i)$

Justification of the error:

- ① It is equivalent to the error propagation formula for  $N \rightarrow \infty$  ( $N$  large)
- ② It provides a stable method to estimate the error even if  $N$  is not large

Proof of ① (exercise):

note that 
$$\bar{f}_i = \frac{1}{N-1} \sum_{\substack{j=1 \\ j \neq i}}^N f(x_j) = \bar{f} + \underbrace{\frac{1}{N-1} (\bar{f} - f(x_i))}_{\Delta}$$

$\Delta$  is small so that

$$J(\bar{f}_i) = J(\bar{f}) + J'(\bar{f}) \Delta_i + \text{negligible terms.}$$

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# DEFINITION OF THE AVERAGE: MOTIVATIONS

⑤

$$\text{ext. } [J(\langle f \rangle_\pi)] = NJ(\bar{f}) - \frac{N-1}{N} \sum_{i=1}^N J(\bar{f}_i)$$

$$\begin{aligned} \bullet \langle J(\bar{f}) \rangle_{MC} &= J(\langle f \rangle_\pi) + \frac{1}{2N} J''(\langle f \rangle_\pi) \text{Var}_\pi f + O(N^{-2}) \\ &= J(\langle f \rangle_\pi) + \frac{a}{N} + O(N^{-2}) \end{aligned}$$

$$\bullet \langle J(\bar{f}_i) \rangle_{MC} = J(\langle f \rangle_\pi) + \frac{a}{N-1} + O(N^{-2}) \quad \left[ \begin{array}{l} \text{of course,} \\ \text{independent of } i \end{array} \right]$$

[ $\bar{f}_i$  is indeed a sample mean over  $(N-1)$  measures]

It follows

$$\begin{aligned} &\left\langle NJ(\bar{f}) - \frac{N-1}{N} \sum_{i=1}^N J(\bar{f}_i) \right\rangle_{MC} \\ &= N \left( J(\langle f \rangle_\pi) + \frac{a}{N} \right) - \frac{N-1}{N} \cdot \underset{\substack{\uparrow \\ \text{there are } N \text{ terms in the sum}}}{N} \left( J(\langle f \rangle_\pi) + \frac{a}{N-1} \right) \\ &= NJ(\langle f \rangle_\pi) + a - (N-1) \left[ J(\langle f \rangle_\pi) + \frac{a}{N-1} \right] \\ &= J(\langle f \rangle_\pi) + O(N^{-2}) \end{aligned}$$

The average is defined so as to eliminate the bias of order  $N$