The Jackknife Approach

Jackknife estimators allow to correct for the bias and the error of the bias. The method was introduced in the 1950s in papers by Quenouille and Tukey. The jackknife method is recommended as the standard for error bar calculations. In unbiased situations the jackknife and the usual error bars agree. Otherwise the jackknife estimates are improvements, so that one cannot lose.

The unbiased estimator of the expectation value $\hat{x}$ is

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

Normally bias problems occur when one estimates a non-linear function of $\hat{x}$:

$$\hat{f} = f(\overline{x}) \, .$$

(1)
Typically, the bias is of order $1/N$:

$$bias \left( \bar{f} \right) = \hat{f} - \langle \bar{f} \rangle = \frac{a_1}{N} + \frac{a_2}{N^2} + O\left( \frac{1}{N^3} \right). \tag{2}$$

Unfortunately, we lost the ability to estimate the variance $\sigma^2(\bar{f}) = \sigma^2(f)/N$ via the standard equation

$$s^2(\bar{f}) = \frac{1}{N} s^2(f) = \frac{1}{N (N - 1)} \sum_{i=1}^{N} (f_i - \bar{f})^2, \tag{3}$$

because $f_i = f(x_i)$ is not a valid estimator of $\hat{f}$. Also it is in non-trivial applications almost always a bad idea to to use standard error propagation formulas with the aim to deduce $\Delta \bar{f}$ from $\Delta \bar{x}$. Jackknife methods are not only easier to implement, but also more precise and far more robust.

The error bar problem for the estimator $\bar{f}$ is conveniently overcome by using
jackknife estimators \( \bar{f}^J, f_i^J \), defined by

\[
\bar{f}^J = \frac{1}{N} \sum_{i=1}^{N} f_i^J \quad \text{with} \quad f_i^J = f(x_i^J) \quad \text{and} \quad x_i^J = \frac{1}{N-1} \sum_{k \neq i} x_k . \tag{4}
\]

The estimator for the variance \( \sigma^2(\bar{f}^J) \) is

\[
s_J^2(\bar{f}^J) = \frac{N-1}{N} \sum_{i=1}^{N} (f_i^J - \bar{f}^J)^2 . \tag{5}
\]

Straightforward algebra shows that in the unbiased case the estimator of the jackknife variance (5) reduces to the normal variance (3).

Notably only of order \( N \) (not \( N^2 \)) operations are needed to construct the jackknife averages \( x_i^J, \ i = 1, \ldots, N \) from the original data.