

interval $[x_i, x_{i+1}]$ is of order $f'''(x_i)(\Delta x)^5$, and that the total error in the interval $[a, b]$ associated with Simpson's rule is $O(n^{-4})$.

The error estimates can be extended to two dimensions in a similar manner. The two-dimensional integral of $f(x, y)$ is the volume under the surface determined by $f(x, y)$. In the "rectangular" approximation, the integral is written as a sum of the volumes of parallelograms with cross-sectional area $\Delta x \Delta y$ and a height determined by $f(x, y)$ at one corner. To determine the error, we expand $f(x, y)$ in a Taylor series:

$$f(x, y) = f(x_i, y_i) + \frac{\partial f(x_i, y_i)}{\partial x}(x - x_i) + \frac{\partial f(x_i, y_i)}{\partial y}(y - y_i) + \dots, \quad (11.68)$$

and write the error as

$$\Delta_i = \left[\iint f(x, y) dx dy \right] - f(x_i, y_i) \Delta x \Delta y. \quad (11.69)$$

If we substitute (11.68) into (11.69) and integrate each term, we find that the term proportional to f cancels and the integral of $(x - x_i) dx$ yields $\frac{1}{2}(\Delta x)^2$. The integral of this term with respect to dy gives another factor of Δy . The integral of the term proportional to $(y - y_i)$ yields a similar contribution. Because Δy is also order Δx , the error associated with the intervals $[x_i, x_{i+1}]$ and $[y_i, y_{i+1}]$ is to leading order in Δx :

$$\Delta_i \approx \frac{1}{2} [f'_x(x_i, y_i) + f'_y(x_i, y_i)] (\Delta x)^3. \quad (11.70)$$

We see that the error associated with one parallelogram is order $(\Delta x)^3$. Because there are n parallelograms, the total error is order $n(\Delta x)^3$. However, in two dimensions, $n = A/(\Delta x)^2$, and hence the total error is order $n^{-1/2}$. In contrast, the total error in one dimension is order n^{-1} , as we saw earlier.

The corresponding error estimates for the two-dimensional generalizations of the trapezoidal approximation and Simpson's rule are order n^{-1} and n^{-2} , respectively. In general, if the error goes as order n^{-a} in one dimension, then the error in d dimensions goes as $n^{-a/d}$. In contrast, Monte Carlo errors vary as $n^{-1/2}$ independent of d . Hence, for large enough d , Monte Carlo integration methods will lead to smaller errors for the same choice of n .

APPENDIX 11B: THE STANDARD DEVIATION OF THE MEAN

In Section 11.4 we found empirically that the probable error associated with a single measurement consisting of n samples is σ/\sqrt{n} , where σ is the standard deviation associated with n data points. We derive this relation in the following. The quantity of experimental interest is denoted as x . Consider m sets of measurements each with n samples for a total of mn samples. For simplicity, we will assume that $n \gg 1$. We use the index α to denote a particular measurement and the index i to designate the i th sample within a measurement. We denote $x_{\alpha,i}$ as sample i in the measurement α . The value of a measurement is given by

$$M_\alpha = \frac{1}{n} \sum_{i=1}^n x_{\alpha,i}. \quad (11.71)$$

The mean \bar{M} of the total mn individual samples is given by

$$\bar{M} = \frac{1}{m} \sum_{\alpha=1}^m M_\alpha = \frac{1}{mn} \sum_{\alpha=1}^m \sum_{i=1}^n x_{\alpha,i}. \quad (11.72)$$

The difference between measurement α and the mean of all the measurements is given by

$$e_\alpha = M_\alpha - \bar{M}. \quad (11.73)$$

We can write the variance of the means as

$$\sigma_m^2 = \frac{1}{m} \sum_{\alpha=1}^m e_\alpha^2. \quad (11.74)$$

We now wish to relate σ_m to the variance of the individual measurements. The discrepancy $d_{\alpha,i}$ between an individual sample $x_{\alpha,i}$ and the mean is given by

$$d_{\alpha,i} = x_{\alpha,i} - \bar{M}. \quad (11.75)$$

Hence, the variance σ^2 of the mn individual samples is

$$\sigma^2 = \frac{1}{mn} \sum_{\alpha=1}^m \sum_{i=1}^n d_{\alpha,i}^2. \quad (11.76)$$

We write

$$e_\alpha = M_\alpha - \bar{M} = \frac{1}{n} \sum_{i=1}^n (x_{\alpha,i} - \bar{M}) \quad (11.77a)$$

$$= \frac{1}{n} \sum_{i=1}^n d_{\alpha,i}. \quad (11.77b)$$

If we substitute (11.77b) into (11.74), we find

$$\sigma_m^2 = \frac{1}{m} \sum_{\alpha=1}^m \left(\frac{1}{n} \sum_{i=1}^n d_{\alpha,i} \right) \left(\frac{1}{n} \sum_{j=1}^n d_{\alpha,j} \right). \quad (11.78)$$

The sum in (11.78) over samples i and j in set α contains two kinds of terms—those with $i = j$ and those with $i \neq j$. We expect that $d_{\alpha,i}$ and $d_{\alpha,j}$ are independent and equally positive or negative on the average. Hence, in the limit of a large number of measurements, we expect that only the terms with $i = j$ in (11.78) survive, and we write

$$\sigma_m^2 = \frac{1}{mn^2} \sum_{\alpha=1}^m \sum_{i=1}^n d_{\alpha,i}^2. \quad (11.79)$$

If we combine (11.79) with (11.76), we arrive at the result

$$\sigma_m^2 = \frac{\sigma^2}{n}. \quad (11.80)$$