Lesson 15: Numerical Integration II

The errors in the left and right endpoint rules for numerical integration are proportional to $1/N$, where N is the number of subintervals. The width of each subinterval is $h = (b-a)/N$, so the error in these methods scales like h. Thus, if you want to reduce the error in a calculation by a factor of 10^6, you must increase the number of subintervals by a factor of 10^6. This requires 10^6 times as many evaluations of the integrand $f(x)$. This might be fine for simple problems, with simple integrands. But for complicated integrands that require a lot of computer time to evaluate, this can be a problem. In those cases we need a more efficient integration scheme.

The midpoint rule is better than the left or right endpoint rules; the errors in this method are proportional to $1/N^2$, or h^2. With the midpoint rule we can reduce the error by a factor of 10^6 by increasing the number of subintervals by a factor of 1000. This requires "only" 1000 times as many evaluations of $f(x)$. Can we do even better?

1 Errors in the rectangle methods

The error in the left endpoint rule can be understood by considering the integrand $f(x)$ in the ith subinterval, between x_{i-1} and x_i. Expand $f(x)$ in a Taylor series about the left endpoint:

$$f(x) = f(x_{i-1}) + f'(x_{i-1})(x - x_{i-1}) + \frac{1}{2}f''(x_{i-1})(x - x_{i-1})^2 + \cdots \tag{1}$$

Integrating over the subinterval, we find

$$\int_{x_{i-1}}^{x_i} f(x)\,dx = f(x_{i-1})h + \frac{1}{2}f'(x_{i-1})h^2 + \frac{1}{6}f''(x_{i-1})h^3 + \cdots \tag{2}$$

where $h = x_i - x_{i-1}$. The first term on the right–hand side is the approximation used by the left endpoint rule. It differs from the exact answer, on the left–hand side, by terms of order h^2, h^3, *etc.* Thus, for each subinterval, the error in the left endpoint rule is

$$\mathcal{E}_L = \frac{1}{2}f'(x_{i-1})h^2 + \frac{1}{6}f''(x_{i-1})h^3 + \cdots \tag{3}$$

The leading term, which dominates for small h, is proportional to h^2. Since there are N subintervals, and N is proportional to $1/h$, the total error in the left–endpoint rule is proportional to $Nh^2 \sim h$.

We can apply a similar argument for the right endpoint rule. Expand $f(x)$ in a Taylor series about the right endpoint,

$$f(x) = f(x_i) + f'(x_i)(x - x_i) + \frac{1}{2} f''(x_i)(x - x_i)^2 + \cdots \tag{4}$$

and integrate to obtain

$$\int_{x_{i-1}}^{x_i} f(x)\, dx = f(x_i)h - \frac{1}{2} f'(x_i)h^2 + \frac{1}{6} f''(x_i)h^3 + \cdots \tag{5}$$

The first term on the right–hand side is the approximation used by the right endpoint rule. Thus the error in the right endpoint rule is

$$\mathcal{E}_R = -\frac{1}{2} f'(x_i)h^2 + \frac{1}{6} f''(x_i)h^3 + \cdots \tag{6}$$

which is proportional to h^2. The total error for N subintervals is $Nh^2 \sim h$.

For the midpoint rule, we expand $f(x)$ in a Taylor series about the midpoint. For notational simplicity, let $x_{i-1/2} \equiv (x_i + x_{i-1})/2$ denote the midpoint. Then

$$f(x) = f(x_{i-1/2}) + f'(x_{i-1/2})(x - x_{i-1/2}) + \frac{1}{2} f''(x_{i-1/2})(x - x_{i-1/2})^2 + \cdots \tag{7}$$

and the integral over the subinterval gives

$$\int_{x_{i-1}}^{x_i} f(x)\, dx = f(x_{i-1/2})h + \frac{1}{24} f''(x_{i-1/2})h^3 + \cdots \tag{8}$$

Note the absence of terms proportional to h^2. The first term on the right–hand side is the midpoint rule approximation to the area for the ith subinterval. Thus, the error for the midpoint rule is

$$\mathcal{E}_M = \frac{1}{24} f''(x_{i-1/2})h^3 + \cdots \tag{9}$$

for each subinterval. The total error for N subintervals is $Nh^3 \sim h^2$.

> Exercise 1: Derive the result (8) from Eq. (7).

2 Trapezoid rule

The errors for the left endpoint rule, (3), and the right endpoint rule, (6), are similar. To be precise, the order h^2 terms are the same apart from the overall sign, and the point of evaluation of $f''(x)$. The point of evaluation should not make much difference, assuming h is small. This suggests that the errors in the left and right endpoint rules should be approximately equal in magnitude but opposite in sign. You might have noticed this from working with the left and right endpoint rules in the previous lesson.

This observation leads us to the trapezoid rule for numerical integration. The trapezoid rule is obtained by taking the *average* of the left and right endpoint rules. That is, we approximate the integral

$$I = \int_a^b f(x)\, dx \tag{10}$$

by

$$I_T = \frac{1}{2}\left(I_L + I_R\right) = \sum_{i=1}^{N} \frac{1}{2}\left[f(a+ih-h) + f(a+ih)\right] h \tag{11}$$

Geometrically, the area for each subinterval is approximated as the area of a trapezoid that touches the curve $f(x)$ at both endpoints. Note that the trapezoid rule can be rearranged in this way:

$$I_T = \frac{h}{2}\left[f(a) + f(b)\right] + \sum_{i=1}^{N-1} f(a+ih)h \tag{12}$$

This result is important because it shows that the trapezoid rule requires only $N+1$ evaluations of the function $f(x)$. This is essentially the same as the number of evaluations required for the left endpoint, right endpoint, and midpoint rules, namely N.

The error for the trapezoid rule is just the average of the left and right endpoint rule errors:

$$\begin{aligned}\mathcal{E}_T &= \frac{1}{2}\left(\mathcal{E}_L + \mathcal{E}_R\right) \\ &= \frac{1}{4}\left[f'(x_{i-1}) - f'(x_i)\right] h^2 + \frac{1}{12}\left[f''(x_{i-1}) + f''(x_i)\right] h^3 + \cdots \end{aligned}\tag{13}$$

Let's evaluate this carefully. First, note that the derivative of Eq. (4) gives

$$f'(x) = f'(x_i) + f''(x_i)(x - x_i) + \cdots \tag{14}$$

Evaluating this expression at x_{i-1}, we find

$$f'(x_{i-1}) = f'(x_i) - f''(x_i)h + \cdots \tag{15}$$

With this result, the error in the trapezoid rule becomes

$$\mathcal{E}_T = -\frac{1}{4}f''(x_i)h^3 + \frac{1}{12}\left[f''(x_{i-1}) + f''(x_i)\right] h^3 + \cdots \tag{16}$$

Note that the difference between $f'(x_{i-1})$ and $f'(x_i)$ is of order h. Likewise, one can show that the difference between $f''(x_{i-1})$ and $f''(x_i)$ is of order h. Since the f'' terms in $\mathcal{E}_T$ are already multiplied by h^3, we can replace $f''(x_{i-1})$ with $f''(x_i)$, and absorb the difference into the unwritten terms (the $\cdots$ terms) in Eq. (16). Thus, we have

$$\mathcal{E}_T = -\frac{1}{12}f''(x_i)h^3 + \cdots \tag{17}$$

This is the error in the trapezoid rule for each subinterval. The total error for N subintervals is $Nh^3 \sim h^2$.

Exercise 2: Use the trapezoid rule to approximate $\int_0^{\pi/2} \sin x\, dx$. Find the number of function evaluations required to achieve an error of less than $\pm 10^{-6}$. Do the same for the left endpoint rule, and compare.

3 Simpson's rule

We have now identified two integration methods with errors of order h^2. The midpoint rule has error $\mathcal{E}_M$, from Eq. (9), in each subinterval. The trapezoid rule has error $\mathcal{E}_T$, from Eq. (17), in each subinterval. We can replace $f''(x_{i-1/2})$ with $f''(x-i)$ in Eq. (9), and absorb the difference into the higher–order unwritten terms. We see that, to leading order, $\mathcal{E}_T = -2\mathcal{E}_M$. This suggests that we can define a new integration method as a weighted sum of the midpoint and trapezoid rules, designed to cancel the order h^3 terms in the error. This leads to *Simpson's rule*:

$$I_S = \frac{1}{3} I_T + \frac{2}{3} I_M \tag{18}$$

which can be written explicitly as

$$I_S = \frac{h}{6}\left\{ f(a) + f(b) + 2\sum_{i=1}^{N-1} f(a+ih) + 4\sum_{i=1}^{N} f(a+ih-h/2) \right\} \tag{19}$$

For Simpson's rule, the errors of order h^3 from Eqs. (9) and (17) cancel. A complete analysis shows that the order h^4 terms in the error actually vanish. The leading non–zero term in the error is proportional to h^5. That is, for Simpson's rule, the error in each subinterval is order h^5. The total error for $N \sim 1/h$ subintervals is proportional to $Nh^5 \sim h^4$.

Geometrically, Simpson's rule is obtained by approximating the area in each subinterval as the area under a parabola that matches the function $f(x)$ at each endpoint and at the midpoint. Simpson's rule is more efficient than any of the other integration methods we have discussed. If we want to reduce the error by a factor of 10^6, we must increase the number of subintervals by a factor of $10^{6/4} \approx 32$. Note that Simpson's rule requires $2N+1$ function evaluations. This is roughly twice as many evaluations as our other methods. However, the rapid reduction of error with a relatively small increase in N will usually offset the extra function calls.

Homework: Use Simpson's rule to approximate $\int_0^{\pi/2} \sin x\, dx$. Make a log–log plot of the error as a function of the number of subintervals, and show that the error is proportional to $1/N^4$. Find the number of function evaluations required for Simpson's rule to achieve an error of less than $\pm 10^{-6}$. Compare with the number of function evaluations needed for the left endpoint rule to achieve a comparable error.

Homework: The error function is defined by

$$\operatorname{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \tag{20}$$

Write a code to evaluate the error function using Simpson's rule, and make a plot of $\operatorname{erf}(x)$ versus x for $0 \leq x \leq 3$.