Numerical integration (also known as quadrature)

To numerically integrate a function $f(x)$ on an interval $[a,b]$, one usually uses approximations of the form

$$\int_a^b f(x)\mathrm{d}x \approx w_0 f(x_0) + \cdots + w_n f(x_n) = \sum_{i=0}^{n} w_i f(x_i),$$

where the points x_i and the weights w_i are chosen appropriately.

Comment. Such **quadrature rules** are typically judged by the maximal degree d of polynomials that they can integrate without error. For instance, to correctly integrate constant functions (degree 0 polynomials), the weights need to be such that they add up to $b-a$. (Why?!)

Common quadrature rules include:

- Newton–Cotes rules: equally spaced points x_i

  These are most useful if $f(x)$ is already computed at equally spaced points, or if evaluation is fast.

  There are closed Newton–Cotes rules and open ones. Open means that a and b are not part of the x_i.

- Gaussian quadrature: the x_i are not equally spaced but chosen carefully

  Choosing the x_i is similar to our discussion of Chebyshev nodes in polynomial interpolation.

  Gaussian quadrature is particularly useful if $f(x)$ is expensive to compute.

Comment. In the case of integrable singularities, such as in $\int_0^1 \frac{1}{\sqrt{x}}\mathrm{d}x$, we cannot use closed Newton–Cotes.

Because of time constraints, we will focus on the simplest example of a closed Newton–Cotes rule, namely the trapezoidal rule.

We will then see that combining this with Richardson extrapolation, we can obtain higher order Newton–Cotes rules such as Simpson's rule.

The (composite) trapezoidal rule

Given equally spaced nodes $x_0, x_1, \ldots, x_n$ with $x_0 = a$ and $x_n = b$, we interpolate $f(x)$ on each segment $[x_{i-1}, x_i]$ by a linear function. Writing $h = (b-a)/n$ for the distance between nodes, the resulting integration rule is the following:

(trapezoidal rule) The following is an approximation of order 2:

$$\int_a^b f(x)\mathrm{d}x \approx \frac{h}{2}[f(x_0) + 2f(x_1) + \cdots + 2f(x_{n-1}) + f(x_n)]$$

Why? On each segment $[x_{i-1}, x_i]$, we approximate $f(x)$ by a linear function so that the integral on that segment becomes the area of a trapezoid and we get

$$\int_{x_{i-1}}^{x_i} f(x)\mathrm{d}x \approx \underbrace{\text{width} \cdot \text{average height}}_{\text{area}} = h \cdot \frac{f(x_{i-1}) + f(x_i)}{2} = \frac{h}{2} f(x_{i-1}) + \frac{h}{2} f(x_i).$$

Make a sketch! Adding together the integrals over all segments, each node (except x_0 and x_n) will show up twice (hence the factor of 2 in front of $f(x_1), \ldots, f(x_{n-1})$) and we get the claimed integration rule. The fact that the trapezoidal rule provides an approximation of order 2 is proved in Theorem 131 below.

Sanity check. Note that the weights are $\frac{h}{2}$ for the first and last node, and h for the others. The sum of the weights is $2 \cdot \frac{h}{2} + (n-1) \cdot h = nh = b - a$. That is what we need to integrate constant functions without error. Indeed, from the construction it is clear that the composite trapezoidal rule integrates linear functions exactly.

Armin Straub
straub@southalabama.edu

Theorem 131. (trapezoidal rule with error term) If f is C^2 smooth, then

$$\int_a^b f(x)\mathrm{d}x = \frac{h}{2}[f(x_0) + 2f(x_1) + \cdots + 2f(x_{n-1}) + f(x_n)] - \frac{(b-a)}{12} f''(\xi) h^2$$

for some $\xi \in [a, b]$. In particular, the trapezoidal rule is of order 2.

Proof. On each segment $[x_{i-1}, x_i]$, the error of the interpolation is

$$f(x) = \text{linear approximation } + \frac{1}{2} f''(\xi)(x - x_{i-1})(x - x_i).$$

Hence, when integrating

$$\int_{x_{i-1}}^{x_i} f(x)\mathrm{d}x = \underbrace{\frac{h}{2} f(x_{i-1}) + \frac{h}{2} f(x_i)}_{\text{integral of linear approx.}} + \underbrace{\int_{x_{i-1}}^{x_i} \frac{1}{2} f''(\xi)(x - x_{i-1})(x - x_i)\mathrm{d}x}_{\text{error}_i},$$

so that the error when integrating is

$$\text{error}_i = \frac{1}{2} f''(\psi) \underbrace{\int_{x_{i-1}}^{x_i} (x - x_{i-1})(x - x_i)\mathrm{d}x}_{= \int_0^h x(x-h)\mathrm{d}x = \left[\frac{1}{3}x^3 - \frac{h}{2}x^2\right]_0^h = -\frac{1}{6}h^3} = -\frac{1}{12} f''(\psi) h^3$$

where ψ is some value between x_{i-1} and x_i. Let us briefly justify the "pulling out" of $f''(\xi)$ even though ξ depends on x. Note that $(x - x_{i-1})(x - x_i)$ is always $\leqslant 0$ in the integral and, therefore, does not change sign. This means that the error integral lies between the corresponding integrals where we replace $f''(\xi)$ with its maximum value M and minimum value L; the values M and L no longer depend on x and therefore can be pulled out of the integral. The above computation then shows that error_i is between $-\frac{1}{12}h^3 M$ and $-\frac{1}{12}h^3 L$, hence must be equal to $-\frac{1}{12}h^3 m$ for some $m \in [L, M]$. Since L and M are the minimum and maximum value of f'' on $[x_{i-1}, x_i]$, and since f'' is continuous, it follows that $m = f''(\psi)$ for some ψ.

To get the overall error, we need to add the errors $-\frac{1}{12} f''(\psi_i) h^3$ from each segment $[x_{i-1}, x_i]$, where $i = 1, 2, \ldots, n$ and where $\psi_i \in [x_{i-1}, x_i]$. The result is

$$-\frac{1}{12} f''(\psi_1) h^3 + \cdots + -\frac{1}{12} f''(\psi_n) h^3 = -\frac{nh}{12} \underbrace{\frac{f''(\psi_1) + \cdots + f''(\psi_n)}{n}}_{= \text{average} = f''(\xi)} h^2 = -\frac{b-a}{12} f''(\xi) h^2,$$

where ξ is some value between a and b. □

Comment. A closer inspection of our proof shows that the $f''(\xi)$ in the error formula converges, as $h \to 0$, to the average value of f'' on $[a, b]$. This means that we have a way to obtain an **error estimate** (rather than only an error bound). This observation is also useful because it shows that the error is of a form that allows us to perform Richardson extrapolation.

Advanced comment. Indeed, using the Euler–Maclaurin formula one can show that the error is

$$-\frac{f'(b) - f'(a)}{12} h^2 + \frac{f'''(b) - f'''(a)}{720} h^4 + \ldots - B_{2m} \frac{f^{(2m-1)}(b) - f^{(2m-1)}(a)}{(2m)!} h^{2m} + O(h^6),$$

where the B_{2m} are rational numbers known as Bernoulli numbers (provided, of course, that f is C^{2m-1} smooth). The fact that only even powers of h show up reflects the fact that the trapezoidal rule is symmetric (and therefore correctly integrates $(x-c)^n$ where $c = (a+b)/2$ and n is odd).

Note that this more precise form of the error tells us that the Richardson extrapolation of the trapezoidal rule will be of order 4 (rather than order 3).

Armin Straub
straub@southalabama.edu

Example 132. Use to approximate $\int_1^3 \frac{1}{x} \mathrm{d}x = \log(3) \approx 1.09861$.

(a) Use the trapezoidal rule with $h = 1$.

(b) Use the trapezoidal rule with $h = 1/2$.

(c) Using Richardson extrapolation, combine the previous two approximations to obtain an approximation of higher order. What are absolute and relative error?

Comment. We will see in the next section that this is equivalent to using Simpson's rule!

Solution. Let us write $f(x) = \frac{1}{x}$.

(a) $\int_1^3 f(x)\,\mathrm{d}x \approx \frac{h}{2}[f(1) + 2f(2) + f(3)] = \frac{1}{2}\left[1 + 2 \cdot \frac{1}{2} + \frac{1}{3}\right] = \frac{7}{6} \approx 1.1667$

Comment. Make a sketch! Can you explain why our approximation (for any h) will be an overestimate of the true value of the integral?

(b) $\int_1^3 f(x)\,\mathrm{d}x \approx \frac{h}{2}\left[f(1) + 2f\left(\frac{3}{2}\right) + 2f(2) + 2f\left(\frac{5}{2}\right) + f(3)\right] = \frac{1}{4}\left[1 + 2 \cdot \frac{2}{3} + 2 \cdot \frac{1}{2} + 2 \cdot \frac{2}{5} + \frac{1}{3}\right]$
$= \frac{67}{60} \approx 1.1167$

Comment. Note that the previous error $\left|\log(3) - \frac{7}{6}\right| \approx 0.068$ ($h = 1$) is roughly 3.8 times as large as our current error $\left|\log(3) - \frac{67}{60}\right| \approx 0.018$ ($h = 1/2$). Since $3.8 \approx 4$, this is in line with what we expect from an order 2 method (in general, we can only expect to observe this for sufficiently small h).

(c) Let us write $A(h)$ and $A\left(\frac{h}{2}\right)$ for our two approximations, and A^* for the true value of the integral.

Since $A(h)$ is an approximation of order 2, we expect $A(h) \approx A^* + Ch^2$ for some constant C.

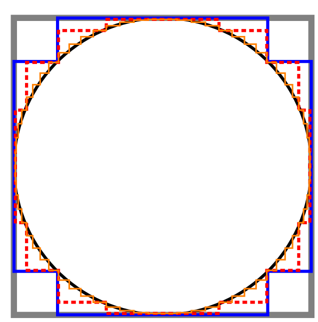
Correspondingly, $A\left(\frac{h}{2}\right) \approx A^* + \frac{1}{4}Ch^2$. Hence, $4A\left(\frac{h}{2}\right) - A(h) \approx (4-1)A^* = 3A^*$.

Therefore, the Richardson extrapolation is $\frac{1}{3}\left[4A\left(\frac{h}{2}\right) - A(h)\right] = \frac{1}{3}\left[4 \cdot \frac{67}{60} - \frac{7}{6}\right] = \frac{11}{10} = 1.1$.

The absolute error is $|1.1 - \log(3)| \approx 0.00139$ and the relative error is $\left|\frac{1.1 - \log(3)}{\log(3)}\right| \approx 0.00126$.

Comment. Note that $\frac{1}{3}\left[4A\left(\frac{h}{2}\right) - A(h)\right] = \frac{h}{3}\left[f(1) + 4f\left(\frac{3}{2}\right) + 2f(2) + 4f\left(\frac{5}{2}\right) + f(3)\right]$. These are the precisely the weights of Simpson's rule.

(Halloween scare!) π is the perimeter of a circle enclosed in a square with edge length 1. The perimeter of the square is 4, which approximates π. To get a better approximation, we "fold" the vertices of the square towards the circle (and get the blue polygon). This construction can be repeated for even better approximations and, in the limit, our shape will converge to the true circle. At each step, the perimeter is 4, so we conclude that $\pi = 4$, contrary to popular belief.



Can you pin-point the fallacy in this argument?

(We are not doing something completely silly! For instance, the areas of our approximations do converge to $\pi/4$, the area of the circle.)

We will talk about a "solution" to the Halloween scare later...