Romberg Integration and Adaptive Quadrature

The goal with both Romberg Integration and Adaptive Quadrature is to increase the accuracy of integration methods while minimizing the amount of extra computations that need to be performed. We begin with Romberg Integration.

Romberg Integration

Romberg integration begins with the Trapezoid Rule:

$$\int_a^b f(x)dx = \frac{h}{2}(f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)) + \text{ error terms.}$$

It can be shown (though we don't) that for an infinitely differentiable function f, the error terms are all constants times the even powers of h. Furthermore, the constants depend only on the derivatives of f at the endpoints (a and b) and not anywhere in the middle. So we have

$$\int_a^b f(x)dx = \frac{h}{2}(f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)) + c_2h^2 + c_4h^4 + c_6h^6 + \cdots .$$

Regarding minimizing the amount of extra computation, we first show that current trapezoid approximations can be used in producing the next approximation when cutting each step size in half. Define the various step sizes, starting with $n = 1$, as follows.

$$\begin{aligned} h_1 &= b - a \\ h_2 &= \frac{1}{2}(b-a) \\ h_3 &= \frac{1}{2^2}(b-a) \\ &\vdots \\ h_j &= \frac{1}{2^{j-1}}(b-a) \end{aligned}$$

So each time we cut the step size in half, we are going from h_j to h_{j+1}. We're going to use the notation R_{j1} and $R_{j+1,1}$ to denote the Trapezoid approximations (the part of F without the error terms) using h_j and h_{j+1}. Looking at the trapezoid rules and rewriting in terms of previous approximations gives the following pattern.

$$\begin{aligned}
R_{11} &= \frac{h_1}{2}(f(a) + f(b)) \\
R_{21} &= \frac{h_2}{2}(f(a) + f(b) + 2f(\frac{a+b}{2})) \\
&= \frac{h_2}{2}(f(a) + f(b)) + h_2(f(\frac{a+b}{2})) \\
&= R_{11} + h_2(f(\frac{a+b}{2})) \\
&\ \ \vdots \\
R_{j1} &= \frac{1}{2}R_{j-1,1} + h_j \sum_{i=1}^{2^{j-2}} f(a + (2i-1)h_j)
\end{aligned}$$

This shows how the previous approximation, $R_{j-1,1}$, can serve as a term in R_{j1}.

The second part of the discussion involves extrapolation. Recall the definition of extrapolation.

Definition 1. The *Richardson extrapolation* or *extrapolation* formula for $F(h)$ is

$$Q \approx \frac{2^n F(\frac{h}{2}) - F(h)}{2^n - 1}.$$

We're considering $F(h) = \frac{h}{2}(f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)) + c_2h^2 + c_4h^4 + c_6h^6 + \cdots$. So to apply extrapolation to the Trapezoid Rule, we need $F(\frac{h}{2}) = F(h_j) = R_{j,1}$. We're going to define $R_{j,k}$ to be the extrapolation of $R_{j,k-1}$ and $R_{j-1,k-1}$. Since $R_{j-1,k-1}$ is order $2(k-1)$, we have

$$\begin{aligned}
R_{j-1,k-1} &= \frac{2^{2(k-1)}R_{j,k-1} - R_{j-1,k-1}}{2^{2(k-1)} - 1} \\
&= \frac{4^{k-1}R_{j,k-1} - R_{j-1,k-1}}{4^{k-1} - 1}
\end{aligned}$$

This creates a table with increasingly more accurate approximations:

$$\begin{array}{llll}
R_{11} & & & \\
R_{21} & R_{22} & & \\
R_{31} & R_{32} & R_{33} & \\
R_{41} & R_{42} & R_{43} & R_{44}
\end{array}$$

where the bottom-right corner is the most accurate approximation at a particular row.

Romberg Integration

$R_{11} = (b-a)\frac{f(a)+f(b)}{2}$

for $j = 2, 3, \ldots$ **do**

$h_j = \frac{b-a}{2^{j-1}}$

$R_{j1} = \frac{1}{2}R_{j-1,1} + h_j \sum_{i=1}^{2^{j-2}} f(a + (2i-1)h_j)$

for k = 2, . . . , j **do**

$R_{jk} = \frac{4^{k-1}R_{j,k-1} - R_{j-1,k-1}}{4^{k-1}-1}$

Example 1. Find R_{33} for $\int_0^1 xe^x dx$. Homework problem asks for R_{55}, so this gets you started.

$R_{11} = \frac{e}{2} \approx 1.359140914229523$

$h_2 = \frac{1}{2}$

$R_{21} = \frac{e}{4} + \frac{1}{2}f(\frac{1}{2}) = \frac{e}{4} + \frac{1}{4}\sqrt{e} \approx 1.091750774789793$

$R_{22} = \frac{4(\frac{e}{4}+\frac{1}{4}\sqrt{e})-\frac{e}{2}}{3} \approx 1.002620728309884$

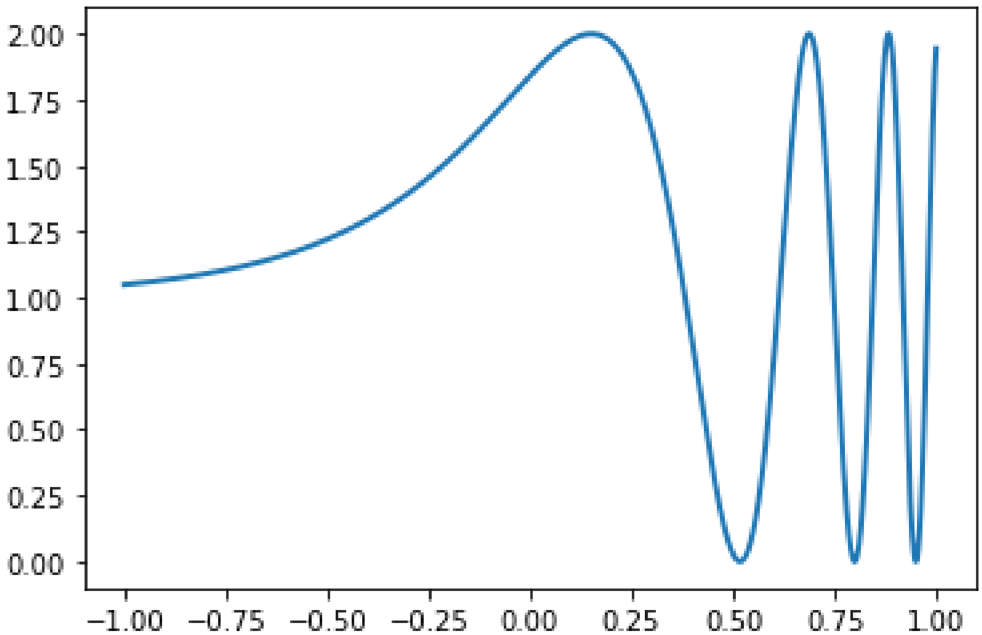
Then $h_3 = \frac{1}{4}$ and $R_{31} = \frac{R_{21}}{2} + \frac{1}{4}(f(\frac{1}{4}) + f(\frac{3}{4})) \approx 1.023064479052757$.

$R_{32} = \frac{4R_{31}-R_{21}}{3} \approx 1.000169047140412$.

$R_{33} = \frac{16R_{32}-R_{22}}{15} \approx 1.000005601729114$.

Adaptive Quadrature

In general, a smaller step size means better approximations for numerical integration. However, some functions might only need a tiny step size in part of the interval, where a lot of change happens, and we can leave a larger step size for the rest. For example, look at the graph of $f(x) = 1 + \sin(e^{3x})$.



We can use the information from the error terms to decide, as we go through the process of dividing the step size by 2, to adapt where we apply a smaller step size.

Start with $[a, b]$. Then $\int_a^b f(x)dx = T_{a,b} - h^3 \frac{f''(c_0)}{12}$.

Now consider splitting the interval $[a, b]$ into $[a, c]$ and $[c, b]$ and using the same formula. Then

$$\begin{aligned}\int_a^b f(x)dx &= T_{a,c} - \frac{h^3}{8}\frac{f''(c_1)}{12} + T_{c,b} - \frac{h^3}{8}\frac{f''(c_2)}{12} \\ &= T_{a,c} + T_{c,b} - \frac{h^3}{4}\frac{f''(c_3)}{12}.\end{aligned}$$

This is the line we should have compared to, not the first one.

Subtracting this from the formula for the $n = 1$ we have

$$T_{a,b} - T_{a,c} - T_{c,b} \approx \frac{3}{4}h^3\frac{f''(c_3)}{12}.$$

Note that the error is about 3 times the error of the previous step, and is computable. So by dividing by 3, we can check if we're within some tolerance of the desired accuracy. If not, subdivide again. But, we can now separately check the error on each subinterval, and stop for intervals that are sufficiently accurate.

I'm not happy with the way the notation played out in the previous version of the algorithm. So instead let's set TOL =(desired accuracy)$\div(b-a)$, the width of the original interval. Then the algorithm is as follows.

Adaptive Quadrature

Set TOL =(desired accuracy)$\div(b-a)$
while not all approximations are sufficiently accurate **do**
  $c = \frac{a+b}{2}$
  $T_{a,b} = (b-a)\frac{f(a)+f(b)}{2}$
  if $|T_{a,b} - T_{a,c} - T_{c,b}| < 3(TOL)(b-a)$ **then**
    accept $T_{a,c} + T_{c,b}$ as approximation over [a,b]
  else
    repeat above recursively for [a,c] and [c,b]

Example 2. Use Adaptive Quadrature to approximate the integral $\int_0^1 x^2 dx$ with TOL = 0.04.

Slight change in desired accuracy so that the decimal numbers in the stopping criteria compare like I wanted :-).

Note that $3(TOL) = 0.12$.

$T_{0,1} = (1)(\frac{0+1}{2}) = \frac{1}{2}$

$c = \frac{1}{2}$

$T_{0,0.5} = \frac{1}{2}(\frac{0+\frac{1}{4}}{2}) = \frac{1}{16}$

$T_{0.5,1} = \frac{1}{2}(\frac{1+\frac{1}{4}}{2}) = \frac{5}{16}$

Then $\frac{1}{2} - \frac{1}{16} - \frac{5}{16} = \frac{1}{8} = 0.125 > (0.12)(1) = 0.12$, so we should continue.

Then $T_{0,0.25} = (\frac{1}{4})\frac{(\frac{1}{16}+0)}{2} = \frac{1}{128}$.

$T_{0.25,0.5} = \frac{5}{128}$.

$T_{0.5,0.75} = \frac{13}{128}$.

$T_{0.75,1} = \frac{25}{128}$.

So $T_{0,0.5} - T_{0,0.25} - T_{0.25,0.5} = \frac{1}{64} \approx 0.016 < 0.12(\frac{1}{2}) = 0.06$ so this interval is sufficiently accurate.

$T_{0.5,1} - T_{0.5,0.75} - T_{0.75,1} = \frac{1}{64} \approx 0.016 < 0.12(\frac{1}{2}) = 0.06$ so this interval is also sufficiently accurate.

Then the final approximation is $T_{0,0.25}+T_{0.25,0.5}+T_{0.5,0.75}+T_{0.75,1} = \frac{1+5+13+25}{128} = \frac{11}{32} = 0.34375$ while the correct answer is $\frac{1}{3} = 0.33333$.

The choice of trapezoid rule only really affects the scalar on the tolerance for the stopping criteria. If using Simpson's Rule instead, the stopping criteria should be

$$|S_{a,b} - S_{a,c} - S_{c,b}| < 15 * TOL,$$

although sometimes 15 is replaced with 10 to make the algorithm more conservative.