2003/10/24 **M174 : Numerical Methods in Science and Engineering**
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§5.2 Trapezoid Rule (continued)

Recall the setting: we are trying to approximate the integral

$$\int_a^b f(x)\mathrm{d}x,$$

for some unpleasant or black box function $f(x)$; we *cannot* just find some antiderivative of $f(x)$ and use the Fundamental Theorem of Calculus.

The Trapezoid Rule approximation of the integral, for a partition with n equal subintervals is

$$\int_a^b f(x)\mathrm{d}x \approx \frac{h}{2}\sum_{i=0}^{n-1} f(x_i)+f(x_{i+1}) = \frac{h}{2}\left[f(x_0)+f(x_1)+f(x_1)+f(x_2)+\ldots+f(x_{n-1})+f(x_n)\right],$$

where $h = (b-a)/n$. Remember the error theorem:

Theorem 1 (Error of the Trapezoid Rule). Let $f''(x)$ be continuous on $[a,b]$. Let T be the value of the trapezoid rule applied to $f(x)$ on this interval with a partition of uniform spacing, h, and let $I = \int_a^b f(x)\mathrm{d}x$. Then there is some $\xi \in [a,b]$ such that

$$I - T = -\frac{(b-a)\,h^2}{12} f''(\xi).$$

Using the Error Bound (again)

Consider the following examples:

Example 2. How many intervals are required to approximate the integral

$$\int_0^2 x^3 - 1\,\mathrm{d}x$$

to within 1×10^{-6}?
We have $f(x) = x^3 - 1$, thus $f'(x) = 3x^2$, and $f''(x) = 6x$. Thus $f''(\xi)$ is continuous and bounded by 12 on $[0,2]$. If we use n equal subintervals then the Trapezoid Error theorem tells us our error will be

$$-\frac{2-0}{12}\left(\frac{2-0}{n}\right)^2 f''(\xi) = -\frac{2f''(\xi)}{3n^2}.$$

To make this smaller than 1×10^{-6}, in absolute value, it suffices to take

$$\frac{24}{3n^2} \le 1 \times 10^{-6},$$

and so $n \ge \sqrt{8} \times 10^3$ suffices. Because $f''(x)$ is positive on this interval, the Trapezoid Rule will be an overestimate.

§5.3 Romberg Algorithm

The error theorem tells us, approximately, that the error of the Trapezoid Rule approximation is $\mathcal{O}\left(h^2\right)$. If we halve h, our error is quartered. Sometimes we want to do better than this. We'll use the same trick that we did from Richardson extrapolation. In fact, the forms are exactly the same.

Towards this end, suppose that f, a, b are given. For a given n, we are going to use the Trapezoid Rule on a partition of 2^n equal subintervals of $[a, b]$. That is $h = \frac{b-a}{2^n}$. Then define

$$\begin{aligned} \phi(n) &= \frac{1}{2}\frac{b-a}{2^n}\sum_{i=0}^{2^n-1} f(x_i) + f(x_{i+1}) \\ &= \frac{b-a}{2^n}\left[\frac{f(a)}{2} + \frac{f(b)}{2} + \sum_{i=1}^{2^n-1} f\left(a + i\frac{b-a}{2^n}\right)\right]. \end{aligned}$$

The intervals used to calculate $\phi(n+1)$ are half the size of those for $\phi(n)$. As mentioned above, this means the error is one quarter.

It turns out that if we had done our error theorem differently, we would have come up with the relation:

$$\phi(n) = \int_a^b f(x)\mathrm{d}x + a_2h_n^2 + a_4h_n^4 + a_6h_n^6 + a_8h_n^8 + \dots,$$

where $h_n = \frac{b-a}{2^n}$. The constants a_i are a function of $f^{(i)}(x)$ only. This should look just like what we did on October 13. (In fact, I am doing a lot of cutting and pasting here) What happens if we now calculate $\phi(n+1)$? We have

$$\begin{aligned} \phi(n+1) &= \int_a^b f(x)\mathrm{d}x + a_2h_{n+1}^2 + a_4h_{n+1}^4 + a_6h_{n+1}^6 + a_8h_{n+1}^8 + \dots, \\ &= \int_a^b f(x)\mathrm{d}x + \frac{1}{4}a_2h_n^2 + \frac{1}{16}a_4h_n^4 + \frac{1}{64}a_6h_n^6 + \frac{1}{256}a_8h_n^8 + \dots. \end{aligned}$$

This happens because $h_{n+1} = \frac{b-a}{2^{n+1}} = \frac{1}{2}\frac{b-a}{2^n} = \frac{h_n}{2}$. As with Richardon's method for approximating derivatives, we now combine the right multiples of these:

$$\begin{aligned} \phi(n) - 4\phi(n+1) &= -3\int_a^b f(x)\mathrm{d}x + \frac{3}{4}4h_n^4 + \frac{15}{16}a_6h_n^6 + \frac{63}{64}a_8h_n^8 + \dots \\ \frac{4\phi(n) - \phi(n+1)}{3} &= \int_a^b f(x)\mathrm{d}x - \frac{1}{4}4h_n^4 - \frac{5}{16}a_6h_n^6 - \frac{21}{64}a_8h_n^8 + \dots \end{aligned}$$

This approximation has a truncation error of $\mathcal{O}\left(h_n^4\right)$.

Like in Richardson's method, we can use this to get better and better approximations to the integral. We do this by constructing a triangular array of approximations, each entry depending on two others. Towards this end, we let

$$R(n, 0) = \phi(n),$$

then define

$$R(n,m) = \frac{4^m R(n,m-1) - R(n-1,m-1)}{4^m - 1}.$$

The familiar pyramid table then is:

$$\begin{array}{lllll}
R(0,0) & & & & \\
R(1,0) & R(1,1) & & & \\
R(2,0) & R(2,1) & R(2,2) & & \\
\vdots & \vdots & \vdots & \ddots & \\
R(n,0) & R(n,1) & R(n,2) & \cdots & R(n,n)
\end{array}$$

Even though this is *exactly* the same as Richardon's method, it has another name: this is called the Romberg Algorithm.

Example 3. Approximating the integral

$$\int_0^2 \frac{1}{1+x^2} \mathrm{d}x$$

by Romberg's Algorithm, find $R(1,1)$.
The first column is calculated by the Trapezoid Rule. Successive columns are found by combining members of previous columns. So we first calculate $R(0,0)$ and $R(1,0)$. These are fairly simple, the first is the Trapezoid Rule on a single subinterval, the second is the Trapezoid Rule on two subintervals. Then

$$\begin{aligned}
R(0,0) &= \frac{2-0}{1}\frac{1}{2}\left[f(0)+f(2)\right] = \frac{6}{5}, \\
R(1,0) &= \frac{2-0}{2}\frac{1}{2}\left[f(0)+f(1)+f(1)+f(2)\right] = \frac{11}{10}.
\end{aligned}$$

Then, using Romberg's Algorithm we have

$$R(1,1) = \frac{4R(1,0) - R(0,0)}{4-1} = \frac{\frac{44}{10} - \frac{12}{10}}{3} = \frac{32}{30} = 1.0\bar{6}.$$

At this point we are tempted to use Richardson's analysis. This would claim that $R(n,n)$ is a $\mathcal{O}\left(h_0^{2(n+1)}\right)$ approximation to the integral. However, $h_0 = b - a$, and need not be smaller than 1. This is a bit different from Richardson's method, where the original h is independently set before starting the triangular array; for Romberg's algorithm, h_0 is determined by a and b.

We can easily deal with this problem by picking some k such that $\frac{b-a}{2^k}$ is small enough, say smaller than 1. Then calculating the following array:

$$\begin{array}{lllll}
R(k,0) & & & & \\
R(k+1,0) & R(k+1,1) & & & \\
R(k+2,0) & R(k+2,1) & R(k+2,2) & & \\
\vdots & \vdots & \vdots & \ddots & \\
R(k+n,0) & R(k+n,1) & R(k+n,2) & \cdots & R(k+n,n)
\end{array}$$

Quite often Romberg's Algorithm is used to compute columns of this array. Subtractive cancelling or unbounded higher derivatives of $f(x)$ can make successive approximations *less* accurate. For this reason, entries in ever rightward columns are usually not calculated, rather lower entries in a single column are calculated instead. That is, the user calculates the array:

$$\begin{array}{ccccc}
R(k,0) & & & & \\
R(k+1,0) & R(k+1,1) & & & \\
R(k+2,0) & R(k+2,1) & R(k+2,2) & & \\
\vdots & \vdots & \vdots & \ddots & \\
R(k+n,0) & R(k+n,1) & R(k+n,2) & \cdots & R(k+n,n) \\
R(k+n+1,0) & R(k+n+1,1) & R(k+n+1,2) & \cdots & R(k+n+1,n) \\
R(k+n+2,0) & R(k+n+2,1) & R(k+n+2,2) & \cdots & R(k+n+2,n) \\
R(k+n+3,0) & R(k+n+3,1) & R(k+n+3,2) & \cdots & R(k+n+3,n) \\
\vdots & \vdots & \vdots & & \vdots
\end{array}$$

Then $R(k+n+l,n)$ makes a fine approximation to the integral as $l \to \infty$. Usually n is small, like 2 or 3.

Recursive Trapezoid Rule

It turns out there is an efficient way of calculating $R(n+1,0)$ given $R(n,0)$; first notice from the above example that

$$\begin{aligned}
R(0,0) &= \frac{b-a}{1}\frac{1}{2}\left[f(a)+f(b)\right], \\
R(1,0) &= \frac{b-a}{2}\frac{1}{2}\left[f(a)+f(\frac{a+b}{2})+f(\frac{a+b}{2})+f(b)\right].
\end{aligned}$$

It would be best to calculate $R(1,0)$ without recalculating $f(a)$ and $f(b)$. It turns out this is possible. Let $h_n = \frac{b-a}{2^n}$, and recall that

$$R(n,0) = \phi(n) = h_n\left[\frac{f(a)+f(b)}{2} + \sum_{i=1}^{2^n-1} f\left(a+ih_n\right)\right].$$

Thus

$$\begin{aligned}
R(n+1,0) = \phi(n+1) &= h_{n+1}\left[\frac{f(a)+f(b)}{2} + \sum_{i=1}^{2^{n+1}-1} f\left(a+ih_{n+1}\right)\right], \\
&= \frac{1}{2}h_n\left[\frac{f(a)+f(b)}{2} + \sum_{i=1}^{2^n-1} f\left(a+(2i-1)h_{n+1}\right) + f\left(a+(2i)\frac{1}{2}h_n\right)\right], \\
&= \frac{1}{2}h_n\left[\frac{f(a)+f(b)}{2} + \sum_{i=1}^{2^n-1} f\left(a+ih_n\right) + \sum_{i=1}^{2^n-1} f\left(a+(2i-1)h_{n+1}\right)\right], \\
&= \frac{1}{2}R(n,0) + h_{n+1}\sum_{i=1}^{2^n-1} f\left(a+(2i-1)h_{n+1}\right).
\end{aligned}$$

Then calculating $R(n+1,0)$ requires only 2^n-1 additional evaluations of $f(x)$, instead of the $2^{n+1}+1$ usually required.