Jim Lambers
MAT 460/560
Fall Semeseter 2009-10
Lecture 29 Notes

These notes correspond to Section 4.5 in the text.

Romberg Integration

Richardson extrapolation is not only used to compute more accurate approximations of derivatives, but is also used as the foundation of a numerical integration scheme called *Romberg integration*. In this scheme, the integral

$$I(f) = \int_a^b f(x)\,dx$$

is approximated using the Composite Trapezoidal Rule with step sizes $h_k = (b-a)2^{-k}$, where k is a nonnegative integer. Then, for each k, Richardson extrapolation is used $k-1$ times to previously computed approximations in order to improve the order of accuracy as much as possible.

More precisely, suppose that we compute approximations $T_{1,1}$ and $T_{2,1}$ to the integral, using the Composite Trapezoidal Rule with one and two subintervals, respectively. That is,

$$\begin{aligned} T_{1,1} &= \frac{b-a}{2}[f(a) + f(b)] \\ T_{2,1} &= \frac{b-a}{4}\left[f(a) + 2f\left(\frac{a+b}{2}\right) + f(b)\right]. \end{aligned}$$

Suppose that f has continuous derivatives of all orders on $[a,b]$. Then, the Composite Trapezoidal Rule, for a general number of subintervals n, satisfies

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] + \sum_{i=1}^{\infty} K_i h^{2i},$$

where $h = (b-a)/n$, $x_j = a + jh$, and the constants $\{K_i\}_{i=1}^{\infty}$ depend only on the derivatives of f. It follows that we can use Richardson Extrapolation to compute an approximation with a higher order of accuracy. If we denote the exact value of the integral by $I(f)$ then we have

$$\begin{aligned} T_{1,1} &= I(f) + K_1 h^2 + O(h^4) \\ T_{2,1} &= I(f) + K_1 (h/2)^2 + O(h^4) \end{aligned}$$

Neglecting the $O(h^4)$ terms, we have a system of equations that we can solve for K_1 and $I(f)$. The value of $I(f)$, which we denote by $T_{2,2}$, is an improved approximation given by

$$T_{2,2} = T_{2,1} + \frac{T_{2,1} - T_{1,1}}{3}.$$

It follows from the representation of the error in the Composite Trapezoidal Rule that $I(f) = T_{2,2} + O(h^4)$.

Suppose that we compute another approximation $T_{3,1}$ using the Composite Trapezoidal Rule with 4 subintervals. Then, as before, we can use Richardson Extrapolation with $T_{2,1}$ and $T_{3,1}$ to obtain a new approximation $T_{3,2}$ that is fourth-order accurate. Now, however, we have two approximations, $T_{2,2}$ and $T_{3,2}$, that satisfy

$$\begin{aligned} T_{2,2} &= I(f) + \tilde{K}_2 h^4 + O(h^6) \\ T_{3,2} &= I(f) + \tilde{K}_2 (h/2)^4 + O(h^6) \end{aligned}$$

for some constant $\tilde{K}_2$. It follows that we can apply Richardson Extrapolation to these approximations to obtain a new approximation $T_{3,3}$ that is *sixth-order* accurate. We can continue this process to obtain as high an order of accuracy as we wish. We now describe the entire algorithm.

Algorithm (Romberg Integration) Given a positive integer J, an interval $[a,b]$ and a function $f(x)$, the following algorithm computes an approximation to $I(f) = \int_a^b f(x)\,dx$ that is accurate to order $2J$.

$h = b - a$
for $j = 1, 2, \ldots, J$ **do**
  $T_{j,1} = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{2^{j-1}-1} f(a+jh) + f(b)\right]$ (Composite Trapezoidal Rule)
  for $k = 2, 3, \ldots, j$ **do**
    $T_{j,k} = T_{j,k-1} + \frac{T_{j,k-1} - T_{j-1,k-1}}{4^{k-1}-1}$ (Richardson Extrapolation)
  end
  $h = h/2$
end

It should be noted that in a practical implementation, $T_{j,1}$ can be computed more efficiently by using $T_{j-1,1}$, because $T_{j-1,1}$ already includes more than half of the function values used to compute $T_{j,1}$, and they are weighted correctly relative to one another. It follows that for $j > 1$, if we split the summation in the algorithm into two summations containing odd- and even-numbered terms, respectively, we obtain

$$\begin{aligned} T_{j,1} &= \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{2^{j-2}} f(a+(2j-1)h) + 2\sum_{j=1}^{2^{j-2}-1} f(a+2jh) + f(b)\right] \\ &= \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{2^{j-2}-1} f(a+2jh) + f(b)\right] + \frac{h}{2}\left[2\sum_{j=1}^{2^{j-2}} f(a+(2j-1)h)\right] \\ &= \frac{1}{2}T_{j-1,1} + h\sum_{j=1}^{2^{j-2}} f(a+(2j-1)h). \end{aligned}$$

Example We will use *Romberg integration* to obtain a sixth-order accurate approximation to

$$\int_0^1 e^{-x^2}\,dx,$$

an integral that *cannot* be computed using the Fundamental Theorem of Calculus. We begin by using the Trapezoidal Rule, or, equivalently, the Composite Trapezoidal Rule

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\left[f(a) + \sum_{j=1}^{n-1} f(x_j) + f(b)\right], \quad h = \frac{b-a}{n}, \quad x_j = a + jh,$$

with $n = 1$ subintervals. Since $h = (b-a)/n = (1-0)/1 = 1$, we have

$$R_{1,1} = \frac{1}{2}[f(0) + f(1)] = 0.68393972058572,$$

which has an absolute error of 6.3×10^{-2}.

If we bisect the interval $[0, 1]$ into two subintervals of equal width, and approximate the area under e^{-x^2} using two trapezoids, then we are applying the Composite Trapezoidal Rule with $n = 2$ and $h = (1-0)/2 = 1/2$, which yields

$$R_{2,1} = \frac{0.5}{2}[f(0) + 2f(0.5) + f(1)] = 0.73137025182856,$$

which has an absolute error of 1.5×10^{-2}. As expected, the error is reduced by a factor of 4 when the step size is halved, since the error in the Composite Trapezoidal Rule is of $O(h^2)$.

Now, we can use Richardson Extrapolation to obtain a more accurate approximation,

$$R_{2,2} = R_{2,1} + \frac{R_{2,1} - R_{1,1}}{3} = 0.74718042890951,$$

which has an absolute error of 3.6×10^{-4}. Because the error in the Composite Trapezoidal Rule satisfies

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + \sum_{j=1}^{n-1} f(x_j) + f(b)\right] + K_1h^2 + K_2h^4 + K_3h^6 + O(h^8),$$

where the constants K_1, K_2 and K_3 depend on the derivatives of $f(x)$ on $[a, b]$ and are independent of h, we can conclude that $R_{2,1}$ has fourth-order accuracy.

We can obtain a second approximation of fourth-order accuracy by using the Composite Trapezoidal Rule with $n = 4$ to obtain a third approximation of second-order accuracy. We set $h = (1-0)/4 = 1/4$, and then compute

$$R_{3,1} = \frac{0.25}{2}\left[f(0) + 2[f(0.25) + f(0.5) + f(0.75)] + f(1)\right] = 0.74298409780038,$$

which has an absolute error of 3.8×10^{-3}. Now, we can apply Richardson Extrapolation to $R_{2,1}$ and $R_{3,1}$ to obtain

$$R_{3,2} = R_{3,1} + \frac{R_{3,1} - R_{2,1}}{3} = 0.74685537979099,$$

which has an absolute error of 3.1×10^{-5}. This significant decrease in error from $R_{2,2}$ is to be expected, since both $R_{2,2}$ and $R_{3,2}$ have fourth-order accuracy, and $R_{3,2}$ is computed using half the step size of $R_{2,2}$.

It follows from the error term in the Composite Trapezoidal Rule, and the formula for Richardson Extrapolation, that

$$R_{2,2} = \int_0^1 e^{-x^2}\,dx + \tilde{K}_2 h^4 + O(h^6), \quad R_{2,2} = \int_0^1 e^{-x^2}\,dx + \tilde{K}_2 \left(\frac{h}{2}\right)^4 + O(h^6).$$

Therefore, we can use Richardson Extrapolation with these two approximations to obtain a new approximation

$$R_{3,3} = R_{3,2} + \frac{R_{3,2} - R_{2,2}}{2^4 - 1} = 0.74683370984975,$$

which has an absolute error of 9.6×10^{-6}. Because $R_{3,3}$ is a linear combination of $R_{3,2}$ and $R_{2,2}$ in which the terms of order h^4 cancel, we can conclude that $R_{3,3}$ is of sixth-order accuracy. $\square$