Richardson Extrapolation

We have seen that the accuracy of methods for computing integrals or derivatives of a function \( f(x) \) depends on the spacing between points at which \( f \) is evaluated, and that the approximation tends to the exact value as this spacing tends to 0.

Suppose that a uniform spacing \( h \) is used. We denote by \( F(h) \) the approximation computed using the spacing \( h \), from which it follows that the exact value is given by \( F(0) \). Let \( p \) be the order of accuracy in our approximation; that is,

\[
F(h) = a_0 + a_1 h^p + O(h^r), \quad r > p,
\]

where \( a_0 \) is the exact value \( F(0) \). Then, if we choose a value for \( h \) and compute \( F(h) \) and \( F(h/q) \) for some positive integer \( q \), then we can neglect the \( O(h^r) \) terms and solve a system of two equations for the unknowns \( a_0 \) and \( a_1 \), thus obtaining an approximation that is \( r \)th order accurate. If we can describe the error in this approximation in the same way that we can describe the error in our original approximation \( F(h) \), we can repeat this process to obtain an approximation that is even more accurate.

This process of extrapolating from \( F(h) \) and \( F(h/q) \) to approximate \( F(0) \) with a higher order of accuracy is called Richardson extrapolation. In a sense, Richardson extrapolation is similar in spirit to Aitken’s \( \Delta^2 \) method, as both methods use assumptions about the convergence of a sequence of approximations to “solve” for the exact solution, resulting in a more accurate method of computing approximations.

Example Consider the function

\[
f(x) = \frac{\sin^2 \left( \frac{\sqrt{x^2 + 1}}{\cos x - x} \right)}{\sin \left( \frac{\sqrt{x^2 - 1}}{\sqrt{x^2 + 1}} \right)}.
\]

Our goal is to compute \( f'(0.25) \) as accurately as possible. Using a centered difference approximation,

\[
f'(x) = \frac{f(x + h) - f(x - h)}{2h} + O(h^2),
\]

with \( x = 0.25 \) and \( h = 0.01 \), we obtain the approximation

\[
f'(0.25) \approx \frac{f(0.26) - f(0.24)}{0.02} = -9.06975297890147,
\]
which has absolute error $3.0 \times 10^{-3}$, and if we use $h = 0.005$, we obtain the approximation
\[
f'(0.25) \approx \frac{f(0.255) - f(0.245)}{0.01} = -9.06746429492149,
\]
which has absolute error $7.7 \times 10^{-4}$. As expected, the error decreases by a factor of approximately 4 when we halve the step size $h$, because the error in the centered difference formula is of $O(h^2)$.

We can obtain a more accurate approximation by applying Richardson Extrapolation to these approximations. We define the function $N_1(h)$ to be the centered difference approximation to $f'(0.25)$ obtained using the step size $h$. Then, with $h = 0.005$, we have
\[
N_1(h) = -9.06975297890147, \quad N_1(h/2) = -9.06746429492149,
\]
and the exact value is given by $N_1(0) = -9.06669877124279$. Because the error in the centered difference approximation satisfies
\[
N_1(h) = N_1(0) + K_1 h^2 + K_2 h^4 + K_3 h^6 + O(h^8),
\]
where the constants $K_1$, $K_2$ and $K_3$ depend on the derivatives of $f(x)$ at $x = 0.25$, it follows that the new approximation
\[
N_2(h) = N_1(h/2) + \frac{N_1(h/2) - N_1(h)}{2^2 - 1} = -9.06670140026149,
\]
has fourth-order accuracy. Specifically, if we denote the exact value by $N_2(0)$, we have
\[
N_2(h) = N_2(0) + \tilde{K}_2 h^4 + \tilde{K}_3 h^6 + O(h^8),
\]
where the constants $\tilde{K}_2$ and $\tilde{K}_3$ are independent of $h$.

Now, suppose that we compute
\[
N_1(h/4) = \frac{f(x + h/4) - f(x - h/4)}{2(h/4)} = \frac{f(0.2525) - f(0.2475)}{0.005} = -9.06689027527046,
\]
which has an absolute error of $1.9 \times 10^{-4}$, we can use extrapolation again to obtain a second fourth-order accurate approximation,
\[
N_2(h/2) = N_1(h/4) + \frac{N_1(h/4) - N_1(h/2)}{3} = -9.06669893538678,
\]
which has absolute error of $1.7 \times 10^{-7}$. It follows from the form of the error in $N_2(h)$ that we can use extrapolation on $N_2(h)$ and $N_2(h/2)$ to obtain a sixth-order accurate approximation,
\[
N_3(h) = N_2(h/2) + \frac{N_2(h/2) - N_2(h)}{2^4 - 1} = -9.06669877106180,
\]
which has an absolute error of $1.8 \times 10^{-10}$. \qed
The Euler-Maclaurin Expansion

In the previous example, it was stated, without proof, that the error in the centered difference approximation could be expressed as a sum of terms involving even powers of the spacing $h$. We would like to use Richardson Extrapolation to enhance the accuracy of approximate integrals computed using the Composite Trapezoidal Rule, but first we must determine the form of the error in these approximations. We have established that the Composite Trapezoidal Rule is second-order accurate, but if Richardson Extrapolation is used once to eliminate the $O(h^2)$ portion of the error, we do not know the order of what remains.

Suppose that $g(t)$ is differentiable on $(-1, 1)$. From integration by parts, we have

$$\int_{-1}^{1} g(t) \, dt = tg(t) \bigg|_{-1}^{1} - \int_{-1}^{1} tg'(t) \, dt = [g(-1) + g(1)] - \int_{-1}^{1} tg'(t) \, dt.$$ 

The first term on the right side of the equals sign is the basic Trapezoidal Rule approximation of the integral on the left side of the equals sign. The second term on the right side is the error in this approximation. If $g$ is $2k$-times differentiable on $(-1, 1)$, and we repeatedly applying integration by parts, $2k-1$ times, we obtain

$$\int_{-1}^{1} g(t) \, dt - [g(-1) + g(1)] = \left[ q_2(t)g'(t) - q_3(t)g''(t) - \cdots + q_{2k}(t)g^{(2k-1)}(t) \right]_{-1}^{1} - \int_{-1}^{1} q_{2k}(t)g^{(2k)}(t) \, dt,$$

where the sequence of polynomials $q_1(t), \ldots, q_{2k}(t)$ satisfy

$q_1(t) = -t, \quad q_{r+1}(t) = q_r(t), \quad r = 1, 2, \ldots, 2k - 1.$

If we choose the constants of integration correctly, then, because $q_1(t)$ is an odd function, we can ensure that $q_r(t)$ is an odd function if $r$ is odd, and an even function if $r$ is even. Furthermore, we can ensure that $q_r(-1) = q_r(1) = 0$ if $r$ is odd. This yields

$$\int_{-1}^{1} g(t) \, dt - [g(-1) + g(1)] = \sum_{r=1}^{k} q_{2r}(1)[g^{(2r-1)}(1) - g^{(2r-1)}(-1)] - \int_{-1}^{1} q_{2k}(t)g^{(2k)}(t) \, dt.$$

Using this expression for the error in the context of the Composite Trapezoidal Rule, applied to the integral of a $2k$-times differentiable function $f(x)$ on a general interval $[a, b]$, yields the Euler-Maclaurin Expansion

$$\int_{a}^{b} f(x) \, dx = \frac{h}{2} \left[ f(a) + 2 \sum_{i=1}^{n} [f(x_{i-1}) + f(x_i)] + f(b) \right] + \sum_{r=1}^{k} c_r h^{2r} \left[ f^{(2r-1)}(b) - f^{(2r-1)}(a) \right] - \left( \frac{h}{2} \right)^{2k} \sum_{i=1}^{m} \int_{x_{i-1}}^{x_i} q_{2k}(t)f^{(2k)}(x) \, dx,$$
where, for each \( i = 1, 2, \ldots, n \), \( t = -1 + \frac{2}{h}(x - x_{i-1}) \), and the constants
\[
c_r = \frac{q_r(1)}{2^{2r}} = -\frac{B_{2r}}{(2r)!}, \quad r = 1, 2, \ldots, k
\]
are closely related to the Bernoulli numbers \( B_r \).

It can be seen from this expansion that the error \( E_{\text{trap}}(h) \) in the Composite Trapezoidal Rule, like the error in the centered difference approximation of the derivative, has the form
\[
E_{\text{trap}}(h) = K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots + O(h^{2k}),
\]
where the constants \( K_i \) are independent of \( h \), provided that the integrand is at least \( 2k \) times continuously differentiable. This knowledge of the error provides guidance on how Richardson Extrapolation can be repeatedly applied to approximations obtained using the Composite Trapezoidal Rule at different spacings in order to obtain higher-order accurate approximations.

It can also be seen from the Euler-Maclaurin Expansion that the Composite Trapezoidal Rule is particularly accurate when the integrand is a periodic function, of period \( b - a \), as this causes the terms involving the derivatives of the integrand at \( a \) and \( b \) to vanish. Specifically, if \( f(x) \) is periodic with period \( b - a \), and is at least \( 2k \) times continuously differentiable, then the error in the Composite Trapezoidal Rule approximation to \( \int_a^b f(x) \, dx \), with spacing \( h \), is \( O(h^{2k}) \), rather than \( O(h^2) \). It follows that if \( f(x) \) is infinitely differentiable, such as a finite linear combination of sines or cosines, then the Composite Trapezoidal Rule has an exponential order of accuracy, meaning that as \( h \to 0 \), the error converges to zero more rapidly than any power of \( h \).

**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,
\[
T_{1,1} = \frac{b - a}{2} [f(a) + f(b)] \\
T_{2,1} = \frac{b - a}{4} \left[ f(a) + 2f \left( \frac{a + b}{2} \right) + f(b) \right].
\]
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

\[
T_{1,1} = I(f) + K_1 h^2 + O(h^4)
\]

\[
T_{2,1} = I(f) + K_1 (h/2)^2 + O(h^4)
\]

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

\[
T_{2,2} = I(f) + \tilde{K}_2 h^4 + O(h^6)
\]

\[
T_{3,2} = I(f) + \tilde{K}_2 (h/2)^4 + O(h^6)
\]

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
\[ T_{j,k} = T_{j,k-1} + \frac{T_{j,k-1} - T_{j-1,k-1}}{4^{k-1}} \]  
(Richardson Extrapolation) 

end

\[ h = \frac{h}{2} \]
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

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

**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 \( 6.3 \times 10^{-2} \).

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 $1.5 \times 10^{-2}$. 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 $3.6 \times 10^{-4}$. Because the error in the Composite Trapezoidal Rule satisfies

$$\int_a^b f(x) \, dx = \frac{h}{2} \left[ f(a) + \sum_{j=1}^{n-1} f(x_j) + f(b) \right] + K_1 h^2 + K_2 h^4 + K_3 h^6 + O(h^8),$$

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

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

which has an absolute error of $3.8 \times 10^{-3}$. 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 $3.1 \times 10^{-5}$. 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

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

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 $9.6 \times 10^{-6}$. 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. □