1 Numerical integration

Let \( f : [a, b] \to \mathbb{R} \) be a continuous function. Our quest is to approximate the integral

\[
I(f) = \int_a^b f(x) dx
\]  
(1)

and estimate the error.

Let \( n \) be a positive integer. Let

\[
h = \frac{b - a}{n}, \quad x_j = a + jh, \quad f_j = f(x_j), \quad j = 0, 1, 2, \ldots, n.
\]  
(2)

The composite trapezoidal rule is given by

\[
T_h(f) = \frac{1}{2} h \sum_{j=0}^{n-1} (f_j + f_{j+1}).
\]  
(3)

When \( n = 2N \), then the composite Simpson rule is given by

\[
S_h(f) = \frac{1}{3} h \left( f_0 + 4 \sum_{j=1}^{N} f_{2j-1} + 2 \sum_{j=1}^{N-1} f_{2j} + f_n \right).
\]  
(4)

It is possible to give a formula for the error, specifically we have

\[
I - T_h(f) = -\frac{b - a}{12} f^{(2)}(\theta) h^2, \quad f \in C^2([a, b])
\]

and

\[
I - S_h(f) = -\frac{b - a}{180} f^{(4)}(\xi) h^4, \quad f \in C^4([a, b])
\]

for suitable \( \theta \) and \( \xi \) in \([a, b]\). These formulas are useful when we can determine the sign of the derivatives. However, since we do not know \( \theta \) and \( \xi \) and we rarely have enough information to start estimating the size of the error terms we need another approach. Richardson extrapolation is very well suited for this task.
2 Richardson extrapolation

In this section I will try to explain the main idea about Richardson extrapolation. Let $-\infty < a < b < \infty$ and let $f : [a, b] \to \mathbb{R}$ be a function which is infinitely differentiable on $[a, b]$. Let $I(f), N, n, h,$ and $S_h(f)$ be as in the previous section.

Then the following theorem is true.

**Theorem 1.** There exists positive integers $p < q$ and a real constant $\alpha = \alpha(f)$ such that

$$I(f) - S_h(f) = \alpha h^p + O(h^q).$$

(5)

We are not going to prove this theorem, because it is actually pretty difficult. However, it is critical that you learn how to determine $p$ and how to estimate the term $\alpha h^p$.

Suppose, that you have computed two approximations of $I(f)$, specifically $S_h(f)$ and $S_{2h}(f)$.

What can be said about their difference? By Theorem 1 we have

$$I(f) - S_h(f) = \alpha h^p + O(h^q)$$

$$I(f) - S_{2h}(f) = 2^p \alpha h^p + O(h^q)$$

which implies

$$[I(f) - S_{2h}(f)] - [I(f) - S_h(f)]$$

$$= S_h(f) - S_{2h}(f) = (2^p - 1)\alpha h^p + O(h^q)$$

(6)

Now, suppose you actually knew $p$, then you could estimate

$$\alpha h^p$$

simply because

$$\alpha h^p = \frac{S_h(f) - S_{2h}(f)}{2^p - 1} + O(h^q)$$

In other words

$$I(f) = S_h(f) + \alpha h^p + O(h^q) = S_h(f) + \frac{S_h(f) - S_{2h}(f)}{2^p - 1} + O(h^q).$$

Unfortunately, at this point you do not know $p$! What to do about this? You should use equation (6), replacing $h$ with $2h$, which yields

$$S_{2h}(f) - S_{4h}(f) = (2^p - 1)2^p \alpha h^p + O(h^q)$$
It follows, that if $\alpha \neq 0$, then
\[
\frac{S_{2h}(f) - S_{4h}(f)}{S_h(f) - S_{2h}(f)} = 2^p + O(h^q)
\]
Notice, that if $h$ is sufficiently small, then
\[
\frac{S_{2h}(f) - S_{4h}(f)}{S_h(f) - S_{2h}(f)}
\]
should be close equal to one of the numbers
\[
2, 4, 8, 16, 32, \ldots
\]
In short, by comparing the three approximations
\[
S_h(f), \ S_{2h}(f), \text{ and } S_{4h}(f)
\]
it becomes possible to determine the correct value of $p$, and estimate the size of the term
\[
\alpha h^p.
\]
This is the essence of Richardson extrapolation. In practice, many of the function that you encounter are not infinitely differentiable and there might even be points where they cannot be differentiated even once. An example is $f(x) = \sqrt{x}$ which is not differentiable at $x = 0$. However, you can still use this procedure to determine $p$ and estimate the principal error term, i.e. the term $\alpha h^p$, only it is unlikely that $p$ and $q$ will be integers.