Chapter 5: Numerical Differentiation and Integration

In many applications where the exact formula of a function is not explicit, or when the formulas for its derivatives or integrals are not straightforward, numerical differentiation and integration can be applied instead.

1 Big O and small o notation, Taylor expansion

Let h be a variable. When h approaches zero, different powers of h (positive powers) e.g., h^2 and h^5, approach zero at different speed. For example, h^5 approaches zero faster than h^2, which can be observed by

$$\lim_{h\to 0} \frac{h^5}{h^2} \;=\; \lim_{h\to 0} h^3 \;=\; 0.$$

Given a function of h, say $E(h)$, if

$$\lim_{h\to 0} E(h) = 0,$$

then we can compare the speed of approaching 0 by $E(h)$ with the speed of approaching zero by a certain positive powers of h. If there exists a positive number p, such that

$$\lim_{h\to 0} \frac{E(h)}{h^p} = C \neq 0,$$

where C is a certain non-zero constant independent of h, then we say that $E(h)$ approach zero at the same speed as h^p, and denote it by

$$E(h) = O(h^p).$$

If there exists a positive number q, such that

$$\lim_{h\to 0} \frac{E(h)}{h^q} = 0,$$

then we say that $E(h)$ approach zero faster than h^q, and denote it by

$$E(h) = o(h^q).$$

For example, the followings are true, as h approaches zero,

$$h^5 = o(h^2), \quad 2h^2 = O(h^2), \quad h^3 + 2h^2 = O(h^2), \quad h^3 + 2h^2 = o(h).$$

We have the following theorem on some algebras of the Big O.

Theorem 1 *Let h approach 0. Let p and q are two positive numbers and $p < q$. Then*

$$O(h^p) + O(h^q) = O(h^p).$$

Proof: Denote $E_p(h) = O(h^p)$ and $E_q(h) = O(h^q)$. Then we know that there exist two nonzero constants C_p and C_q such that

$$\lim_{h\to 0} \frac{E_p(h)}{h^p} = C_p \neq 0, \quad \text{and} \quad \lim_{h\to 0} \frac{E_q(h)}{h^q} = C_q \neq 0.$$

Then

$$\begin{aligned} \lim_{h\to 0} \frac{O(h^p) + O(h^q)}{h^p} &= \lim_{h\to 0} \frac{E_p(h) + E_q(h)}{h^p} = \lim_{h\to 0} \frac{E_p(h)}{h^p} + \lim_{h\to 0} \frac{E_q(h)}{h^p} \\ &= C_p + \lim_{h\to 0} \left(\frac{E_q(h)}{h^q} \cdot \frac{h^q}{h^p} \right) = C_p + 0 = C_p. \qquad \square \end{aligned}$$

From Theorem 2, we have, as h approaches zero,

$$O(h) + O(h^2) + O(h^3) + \ldots = O(h).$$

An important tool is the Taylor's expansion.

Theorem 2 *(Taylor's expansion in one dimension) Let $f(x)$ be a smooth function of x. Given h, the expansion of $f(x+h)$ at the point x is*

$$f(x+h) = f(x) + hf'(x) + \frac{f''(x)}{2}h^2 + \cdots + \frac{f^{(n)}(x)}{n!}h^n + \ldots,$$

which is called the Taylor series.

The Taylor series can be regarded as a sequence of approximations to $f(x+h)$ with increasing accuracy. The error of the approximation given by a number of terms in the Taylor series is called the *Truncation Error*. Here we have

$$f(x+h) = f(x) + hf'(x) + \frac{f''(x)}{2}h^2 + \cdots + \frac{f^{(n)}(x)}{n!}h^n + \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1},$$

where $\xi \in (x, x+h)$. We denote the truncation error by $E(h)$

$$E(h) = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1}.$$

For a fixed n, assume that $|f^{(n+1)}(\xi)/(n+1)!|$ is bounded by a constant independent of h, then we have

$$E(h) = O(h^{n+1}).$$

2 Numerical differentiation

Numerical differentiation gives an estimate of the derivative of a function $f(x)$, by using only the function values at some discrete points. The approach is the following described finite difference formulas.

From

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(\xi)$$

we have

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}f''(\xi) = \frac{f(x+h) - f(x)}{h} + O(h),$$

i.e., the approximation of $f'(x)$ by $(f(x+h) - f(x))/h$ has an error in the order of h. We call this as *forward difference formula*. Graphically, the slope of the tangent line of the function $y = f(x)$ at $(x, f(x))$ is approximated by the slope of the secant line connecting $(x, f(x))$ and $(x+h, f(x+h))$.

Similarly we have the *backward difference formula*

$$f'(x) = \frac{f(x) - f(x-h)}{h} + O(h),$$

which approximates the derivative $f'(x)$ by the slope of the secant line connecting $(x-h, f(x-h))$ and $(x, f(x))$.

Approximating the derivative $f'(x)$ by the slope of the secant line connecting $(x-h, f(x-h))$ and $(x+h, f(x+h))$ generates the following *central difference* formula

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

where the truncation error $O(h^2)$ is derived by subtracting the following two Taylor's expansions

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{3!}f'''(\xi_1), \quad \text{with} \quad \xi_1 \in [x, x+h]$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{3!}f'''(\xi_2), \quad \text{with} \quad \xi_1 \in [x-h, x]$$

In general the central difference formula is more accurate than either the forward or the backward difference formula.

The same idea can be used to approximate the second order derivative $f''(x)$. First apply a *central difference* formula on the first derivatives, and we have

$$f''(x) \approx \frac{f'(x+\frac{h}{2}) - f'(x-\frac{h}{2})}{h},$$

where both $f'(x+h/2)$ and $f'(x-h/2)$ are approximated by central difference formulas,

$$f'(x+\frac{h}{2}) \approx \frac{f(x+h) - f(x)}{h}, \qquad f'(x-\frac{h}{2}) \approx \frac{f(x) - f(x-h)}{h}.$$

Then we have

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

The error for the above approximation can be obtained by Taylor's expansions. Since

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{6}h^3 + \frac{f^{(4)}(\xi_1)}{24}h^4,$$

and

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{6}h^3 + \frac{f^{(4)}(\xi_2)}{24}h^4,$$

we have

$$f(x+h) - 2f(x) + f(x-h) = f''(x)h^2 + \frac{f^{(4)}(\xi)}{12}h^4.$$

Therefore we have

$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - f''(x) = \frac{f^{(4)}(\xi)}{12}h^2 = O(h^2).$$

3 Numerical integration

We discuss the computation of the integral

$$\int_a^b f(x)dx$$

numerically by applying some quadrature rules.

Let us recall the definition of the Riemann integral of a function $f(x)$ on an interval $[a, b]$. It is defined as the limit of the Riemann sums

$$R_n = \sum_{i=0}^{n-1} (x_{i+1} - x_i)\ f(\xi_i),$$

where the discrete points x_i, $i = 0, 1, 2, ..., n$ can be chosen as equally spaced points of the interval $[a, b]$, i.e.,

$$x_i = a + i * h, \quad i = 0, 1, 2, ..., n, \quad \text{with} \quad h = \frac{b-a}{n},$$

and ξ_i is any chosen value on the interval $[x_i,\ x_{i+1}]$. We can see that R_n in fact represents the sum of areas of n rectangles. If the limit of R_n exists, as n goes to infinity, then we say the function $f(x)$ is Riemann integrable on the interval $[a, b]$, and we define that limit as its integral on the interval $[a, b]$, i.e.,

$$\int_a^b f(x)\ dx = \lim_{n\to\infty} R_n = \lim_{n\to\infty} \sum_{i=0}^{n-1} (x_{i+1} - x_i)\ f(\xi_i).$$

If a function $f(x)$ is bounded and continuous on an interval $[a, b]$, then it is Riemann integrable. In the following, we always say $f(x)$ is bounded and continuous.

4 Quadrature rules

We are looking for some methods to compute the definite integral of a function $f(x)$ by using its function values $f(x_i)$ at some nodes x_i on an interval $[a, b]$. Mathematically, we evaluate

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

by a quadrature rule

$$Q_n(f) = \sum_{i=0}^{n} w_i f(x_i),$$

where $a \le x_0 < x_1 < x_2 < ... < x_n \le b$ represents a partition of the interval $[a, b]$. We call each x_i a *node* or a *point*, and w_i the *weight* at the node x_i. Here we assume that these x_i are equally spaced points as mentioned before, i.e.,

$$x_i = a + i * h, \quad i = 0, 1, 2, ..., n, \quad \text{with} \quad h = \frac{b-a}{n}.$$

Riemann sums can in fact be used as quadrature rule. For example, taking $n = 1$, $x_0 = a$, $x_1 = b$, in the Riemann sum, we have the following approximation of the definite integral

$$I(f) = (x_1 - x_0)f(\xi_0),$$

where we can simply take $\xi_0 = x_0 = a$, and we have the following *rectangle* rule:

$$I(f) = (b - a)f(a).$$

A better choice of ξ_0 is $\xi_0 = (a + b)/2$, the middle point of the interval $[a, b]$, which gives us the following *midpoint* rule:

$$M(f) = (b - a)f\left(\frac{a+b}{2}\right).$$

If we take ξ_0 as the the point where $f(\xi_0) = (f(a) + f(b))/2$, ($\xi_0$ must exist from the intermediate value theroem), then we have the following *trapezoid* rule

$$T(f) = (b - a)\left(\frac{1}{2}f(a) + \frac{1}{2}f(b)\right).$$

A combination of $M(f)$ and $T(f)$ as $(2M(f)+T(f))/3$ leads to the following *Simpson's* rule

$$S(f) = (b - a)\left(\frac{1}{6}f(a) + \frac{4}{6}f\left(\frac{a+b}{2}\right) + \frac{1}{6}f(b)\right).$$

In the following, we discuss some more generals ways deriving the quadrature rules.

4.1 Derived from polynomial interpolation

For the rectangle rule, we can think that we first interpolate the function $f(x)$, at the point $[a, f(a)]$ by a polynomial of degree zero, which is $p_0(x) = f(a)$, then we approximate

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

by

$$\int_a^b p_0(x) = \int_a^b f(a) = (b-a)f(a),$$

which gives us the rectangle rule. Since $p_0(x)$ recovers $f(x)$ exactly when $f(x)$ is a polynomial of degree 0, we know the rectangle gives us the exact integral of a function $f(x)$, if $f(x)$ is a polynomial of degree 0.

For the midpoint rule, we can think that we first interpolate the function $f(x)$, at the middle point point $[(a+b)/2, f((a+b)/2)]$ by a polynomial of degree zero, which is $p_0(x) = f((a+b)/2)$, then we approximate the integral by

$$\int_a^b p_0(x) = \int_a^b f((a+b)/2) = (b-a)f\left(\frac{a+b}{2}\right),$$

which gives us the midpoint rule. We also know that the rectangle gives us the exact integral of any function $f(x)$, if $f(x)$ is a polynomial of degree 0. In fact, observed from the graph, for any linear function $f(x)$, i.e., for any polynomial of degree at most one, the midpoint rule gives the exact integral $\int_a^b f(x)\ dx$.

As for the trapezoid rule, we first find the linear interpolation $p_1(x)$ of the function $f(x)$ based on its two end points $[a, f(a)]$ and $[b, f(b)]$,

$$p_1(x) = f(a) + \frac{f(b)-f(a)}{b-a}(x-a),$$

and its integral

$$\begin{aligned}\int_a^b p_1(x) &= (b-a)f(a) + \frac{b^2-a^2}{2}\frac{f(b)-f(a)}{b-a} - (f(b)-f(a))a \\ &= (b-a)\left(\frac{1}{2}f(a) + \frac{1}{2}f(b)\right),\end{aligned}$$

is called the trapezoid rule. We can see that the trapezoid rule is accurate for polynomials of degree at most 1.

The same procedure can be used to derive the Simpson's rule, which results from integrating the interpolation polynomial of degree two through the three interpolation points $[a, f(a)]$, $[(a+b)/2, f((a+b)/2)]$, and $[b, f(b)]$. It can be shown that, for any polynomial of degree at most 3, the Simpson's rule generates the exact integral $\int_a^b f(x)\ dx$. For example, consider that $f(x) = x^3$.

$$\int_a^b f(x)\ dx = \int_a^b x^3\ dx = \frac{b^4-a^4}{4}.$$

Obtained from applying the Simpson's rule on $f(x) = x^3$, is

$$\begin{aligned} S(f) &= (b-a)\left(\frac{1}{6}f(a) + \frac{4}{6}f\left(\frac{a+b}{2}\right) + \frac{1}{6}f(b)\right) = \frac{(b-a)}{6}\left(a^3 + 4\left(\frac{a+b}{2}\right)^3 + b^3\right) \\ &= \frac{(b-a)}{12}\left(2a^3 + a^3 + 3a^2b + 3ab^2 + b^3 + 2b^3\right) = \frac{(b-a)}{4}\left(a^3 + a^2b + ab^2 + b^3\right) \\ &= \frac{b^4 - a^4}{4} = \int_a^b f(x)\, dx. \end{aligned}$$

We say a quadrature rule is of *degree* d, if the quadrature rule gives the exact integral (with no error) for any polynomial of degree at most d, but not exact for some polynomials of degree $d+1$.

4.2 Derived by method of undetermined coefficients

By requiring a quadrature rule to be exact for the first few monomial basis of polynomials, we can also determine the rectangle rule, midpoint rule, trapezoid rule, and Simpson's rule.

For example, if we need to determine a quadrature rule of the form

$$w_1 f(a) + w_2 f\left(\frac{a+b}{2}\right) + w_3 f(b)$$

by requiring it gives the exact integrals for the monomial basis functions 1, x, x^2, then we have

$$\begin{aligned} w_1 \cdot 1 + w_2 \cdot 1 + w_3 \cdot 1 &= \int_a^b 1 \quad dx = b - a \\ w_1 \cdot a + w_2 \cdot \frac{a+b}{2} + w_3 \cdot b &= \int_a^b x \quad dx = \frac{b^2 - a^2}{2} \\ w_1 \cdot a^2 + w_2 \cdot \left(\frac{a+b}{2}\right)^2 + w_3 \cdot b^2 &= \int_a^b x^2 \quad dx = \frac{b^3 - a^3}{3}. \end{aligned}$$

This leads to a linear system for the coefficients w_1, w_2, w_3. By solving this linear system, we obtain

$$w_1 = \frac{b-a}{6}, \quad w_2 = \frac{4(b-a)}{6}, \quad w_1 = \frac{b-a}{6},$$

which is the Simpson's rule.

5 Accuracy of quadrature rules

Taylor series will be used to estimate the error of quadrature rules. Let us look at the rectangle rule first, where

$$I(f) = (b-a)f(a).$$

Expanding $f(x)$ at the point $x = a$, gives us

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \frac{f'''(a)}{6}(x-a)^3 + \dots.$$

Then we have

$$\begin{aligned} \int_a^b f(x) &= \int_a^b \left(f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \frac{f'''(a)}{6}(x-a)^3 + \dots \right) \\ &= (b-a)f(a) + f'(a)\frac{(b-a)^2}{2} + f''(a)\frac{(b-a)^3}{6} + f'''(a)\frac{(b-a)^4}{24} + \dots \end{aligned}$$

we have the error of the rectangle rule as

$$E_I = I(f) - \int_a^b f(x) = -f'(a)\frac{(b-a)^2}{2} - f''(a)\frac{(b-a)^3}{6} - f'''(a)\frac{(b-a)^4}{24} - \dots$$

from which we can see that rectangle rule is accurate for any polynomial of degree 0. We also see that the leading error is of the order $(b-a)^2$, when $b - a < 1$.

To estimate the error for the midpoint rule,

$$M(f) = (b-a)f\left(\frac{a+b}{2}\right),$$

we expand $f(x)$ at the point $(a+b)/2$. We have

$$f(x) = f\left(\frac{a+b}{2}\right) + f'\left(\frac{a+b}{2}\right)\left(x - \frac{a+b}{2}\right) + \frac{f''(\frac{a+b}{2})}{2}\left(x - \frac{a+b}{2}\right)^2 + \frac{f'''(\frac{a+b}{2})}{6}\left(x - \frac{a+b}{2}\right)^3 + \dots.$$

Since

$$\int_a^b \left(x - \frac{a+b}{2}\right) = 0, \quad \int_a^b \left(x - \frac{a+b}{2}\right)^3 = 0, \quad (\text{ called as } \textit{symmetry} \text{ }),$$

we have

$$\begin{aligned} \int_a^b f(x) &= \int_a^b \left(f\left(\frac{a+b}{2}\right) + \frac{f''(\frac{a+b}{2})}{2}\left(x - \frac{a+b}{2}\right)^2 + \frac{f^{(4)}(\frac{a+b}{2})}{24}\left(x - \frac{a+b}{2}\right)^4 + \dots \right) \\ &= (b-a)f\left(\frac{a+b}{2}\right) + \frac{f''(\frac{a+b}{2})}{24}(b-a)^3 + \frac{f^{(4)}(\frac{a+b}{2})}{1920}(b-a)^5 + \dots \end{aligned}$$

We have the error of the midpoint rule as

$$E_M = M(f) - \int_a^b f(x) = \frac{f''(\frac{a+b}{2})}{24}(b-a)^3 + \frac{f^{(4)}(\frac{a+b}{2})}{1920}(b-a)^5 + \dots$$

from which we can see that midpoint rule is accurate for any polynomial of degree 1. We also see that the error is in the order of $(b-a)^3$.

The same procedure can be applied to the trapezoid rule and the Simpson's rule, and we have

$$E_T = T(f) - \int_a^b f(x) = O\left((b-a)^3\right),$$

for the trapezoid rule, and

$$E_S = S(f) - \int_a^b f(x) = O\left((b-a)^5\right),$$

for the Simpson's rule.

In general, let us denote a $n+1$-point quadrature rule as

$$Q_n(f) = \sum_{i=0}^{n} w_i f(x_i).$$

We have mentioned that the quadrature rule can be determined by first interpolating the points $[x_i, f(x_i)]$, $i = 0, 1, 2, ..., n$, by a polynomial $p_n(x)$, of degree at most n, and then compute the integral of $p_n(x)$. The error of the quadrature rule can then be determined by

$$\left| \int_a^b f(x) - Q_n(f) \right| = \left| \int_a^b f(x) - \int_a^b p_n(x) \right| \le (b-a)\ \|f(x) - p_n(x)\|_\infty$$

From the accuracy of polynomial interpolation, we know that

$$f(x) - p_n(x) \ = \ \frac{f^{(n+1)}(\xi)}{(n+1)!}\ (x-x_0)\ (x-x_1)\ (x-x_2)\ ...\ (x-x_n).$$

Assume that x_i, $i = 0, 1, 2, ..., n$ are equally spaced points on the interval $[a, b]$, i.e., $x_i = a + i * h$, with $h = (b-a)/n$. Then we have

$$\|f(x) - p_n(x)\|_\infty \ \le \ \frac{\|f^{(n+1)}(x)\|_\infty}{(n+1)!} h^{n+1} n!.$$

Therefore

$$\left| \int_a^b f(x) - Q_n(f) \right| \le (b-a)\ \|f(x)-p_n(x)\|_\infty \le (b-a)\ \frac{\|f^{(n+1)}(x)\|_\infty}{n+1} h^{n+1} \ \le \ h^{n+2} \|f^{(n+1)}(x)\|_\infty.$$

We can see that the error will reduce with the decrease of h, i.e., with the increase of the number of points used in the partition. However, when n is large, high order polynomial interpolation will be used for the quadrature rule, which will become ill conditioned as we discussed before. A common approach to fix this is to subdivide the interval $[a, b]$ into smaller intervals and then apply lower order quadrature rule on each on subinterval. Such an approach leads to the *composite quadrature* rules discussed below.

6 Composite quadrature rules

Subdivide the interval $[a, b]$ into n subintervals by equally spaced points x_i, $i = 0, 1, 2, ..., n$, where

$$x_i = a + i\ h, \quad i = 0, 1, 2, ..., n, \qquad \text{with} \qquad h = \frac{b-a}{n}.$$

Then we know

$$\int_a^b f(x)\ dx = \left(\int_{x_0}^{x_1} + \int_{x_1}^{x_2} + ... + \int_{x_{n-1}}^{x_n}\right) f(x)\ dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)\ dx.$$

We can then use quadrature rules on each single subinterval $[x_i, x_{i+1}]$ to compute the integral on each subinterval, and compute the sum at the end.

Composite rectangle rule. On each interval $[x_i, x_{i+1}]$, we apply the rectangle rule to approximate the integral, i.e.,

$$\int_{x_i}^{x_{i+1}} f(x) \approx I_{[x_i,x_{i+1}]}(f) = (x_{i+1} - x_i) f(x_i) = h f(x_i).$$

Then the total integral on the whole interval $[a, b]$ is approximated by

$$\begin{aligned}
\int_a^b f(x)\ dx &= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)\ dx \approx \sum_{i=0}^{n-1} I_{[x_i,x_{i+1}]}(f) = \sum_{i=0}^{n-1} h f(x_i) \\
&= h\left(f(x_0) + f(x_1) + \cdots + f(x_{n-1})\right)
\end{aligned}$$

and we call this the composite rectangle rule.

To analyze the error of the composite rectangle rule on the whole interval $[a, b]$, we know that the error of the rectangle rule on each interval $[x_i, x_{i+1}]$ is

$$E_{[x_i,x_{i+1}]} = h f(x_i) - \int_{x_i}^{x_{i+1}} f(x) = O\left((x_{i+1} - x_i)^2\right) = O\left(h^2\right).$$

Then the total error is

$$E_I(h) = \sum_{i=0}^{n-1} \left(h f(x_i) - \int_{x_i}^{x_{i+1}} f(x)\right) = \sum_{i=1}^{n} E_{[x_{i-1},x_i]} = \sum_{i=1}^{n} O\left(h^2\right) = O\left(n\ h^2\right) = O(h).$$

We say the composite rectangle rule is of first order accurate.

Similarly, the other composite quadrature rules can be derived. For example, the composite trapezoid rule is

$$\begin{aligned}
\int_a^b f(x)\ dx &= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)\ dx \approx \sum_{i=0}^{n-1} \frac{h}{2}\left(f(x_i) + f(x_{i+1})\right) \\
&= h\left(\frac{f(x_0)}{2} + f(x_1) + \cdots + f(x_{n-1}) + \frac{f(x_n)}{2}\right).
\end{aligned}$$

The errors can also be derived similarly. For example, for the composite middle point rule,

$$E_M(h) = \sum_{i=1}^{n} O\left(h^3\right) = O\left(n\ h^3\right) = O(h^2),$$

and it is of second order accurate, which is also true for the composite trapezoid rule. For the composite Simpson's rule, we have

$$E_S(h) = \sum_{i=1}^{n} O\left(h^5\right) = O\left(n\ h^5\right) = O(h^4),$$

and it is fourth order accurate.

7 Richardson extrapolation and convergence analysis

Assume that we are computing a value A, which is the exact solution to a problem. For example

$$A = \int_a^b f(x).$$

Suppose, given a step size h, we can find an approximation of A, denoted by $A(h)$. For example $A(h)$ can be the result of composite rectangle rule for computing an integral. Let $E(h)$ represent the error of this approximation, i.e., $E(h) = A(h) - A$. In general we have an *asymptotic error expansion* in powers of h, i.e.,

$$E(h) = \alpha h^{p_1} + \beta h^{p_2} + ...$$

where α and β, etc., are constants independent of h. For example, when we apply the composite rectangle rule to compute $\int_a^b f(x)$, we have $E(h) = O(h) = \alpha h + \beta h^2 + \ldots$

We can then write $A(h)$ as

$$A(h) = A + \alpha h^{p_1} + \beta h^{p_2} + ...$$

If we choose $h/2$ as the step size, we have

$$A(h/2) = A + \alpha \frac{h^{p_1}}{2^{p_1}} + \beta \frac{h^{p_2}}{2^{p_2}} + ...$$

From the above two equations we have

$$A(h) - 2^{p_1} A(h/2) = (A - 2^{p_1} A) + \left(1 - \frac{2^{p_1}}{2^{p_2}}\right) \beta h^{p_2} + ...,$$

which gives

$$A = \frac{A(h) - 2^{p_1} A(h/2)}{1 - 2^{p_1}} + O(h^{p_2}).$$

Let us denote

$$R(h) = \frac{A(h) - 2^{p_1} A(h/2)}{1 - 2^{p_1}},$$

then we have

$$R(h) = A + O(h^{p_2}),$$

$R(h)$ provides an approximation of A with higher accuracy than the original rule $A(h)$. We call such an approach the Richardson extrapolation. It is useful if we know the order of accuracy p_1 of an approximation $A(h)$.

However, in some applications when we find an approximation $A(h)$ of A, the order of accuracy of $A(h)$ may be unknown. In such cases, we can in fact determine its order of accuracy by the approach described below.

Assume we have an algorithm which approximates A by $A(h)$ for each given step size h. Suppose that the error $E(h)$ is the order of p_1, i.e.,

$$E(h) = O(h^{p_1}) \approx C\ h^{p_1},$$

where p_1 may be not available in advance and C is a constant independent of h. Then by computing a sequence of $A(h)$ for different step size h, we can determine p_1 numerically.

Observing

$$E(h) \approx C\ h^{p_1}, \qquad E(h/2) \approx C\ \frac{h^{p_1}}{2^{p_1}},$$

we have

$$\frac{E(h)}{E(h/2)} \approx 2^{p_1}.$$

Therefore, if we know the exact answer A of a problem, then by computing $A(h)$ and $A(h/2)$, and therefore the errors $E(h)$ and $E(h/2)$, we will be able to determine p_1, as above.

However in most applications, the exact solution A is unknown. Then we can consider

$$A(h) = A + E(h) \approx A + C\ h^{p_1},$$

$$A(h/2) = A + E(h/2) \approx A + C\frac{h^{p_1}}{2^{p_1}},$$

$$A(h/4) = A + E(h/4) \approx A + C\frac{h^{p_1}}{4^{p_1}}.$$

Therefore

$$A(h/2) - A(h) \approx C\left(\frac{1}{2^{p_1}} - 1\right) h^{p_1},$$

$$A(h/4) - A(h/2) \approx C\left(\frac{1}{4^{p_1}} - \frac{1}{2^{p_1}}\right) h^{p_1},$$

and then we have

$$\frac{A(h/2) - A(h)}{A(h/4) - A(h/2)} \approx 2^{p_1},$$

which provides an estimate of p_1.

We have to say that these estimate make sense only when the step size h is small enough, since all these $\approx$ are based on the asymptotic expansion of the error, which is accountable only when h is small enough.