5 Numerical Differentiation and Integration

5.1 Numerical differentiation

We begin by approximating the function $f(x)$ by its Lagrange interpolant $L_n(x)$, namely $f(x) \approx L_n(x)$, then obtain an approximation to the derivative by $f'(x) \approx L_n'(x)$. Approximating the derivative by the derivative of the interpolant, we might ask how good is the approximation? We know the error in $L_n(x)$ (using Theoreom I2),

$$f(x) - L_n(x) = \frac{\Pi(x) f^{(n+1)}(\xi(x))}{(n+1)!}.$$

Therefore, differentiating and applying the chain rule gives:

$$\begin{aligned}
f'(x) - L_n'(x) &= \frac{d}{dx}\left(\frac{\Pi(x) f^{(n+1)}(\xi(x))}{(n+1)!}\right) \\
&= \frac{1}{(n+1)!}\frac{d}{dx}(\Pi(x)) f^{(n+1)}(\xi(x)) \\
&+ \frac{\Pi(x)}{(n+1)!}\frac{d}{dx}\left(f^{(n+1)}(\xi(x))\right) \\
&= \frac{1}{(n+1)!}\left(\sum_{j=0}^{n} \Pi_j(x)\right) f^{(n+1)}(\xi(x)) \\
&+ \frac{\Pi(x)}{(n+1)!}\frac{d}{dx}\left(f^{(n+1)}(\xi(x))\right).
\end{aligned}$$

We do not know much about this second term except that it is zero at the interpolation points. Thus, if we approximate the derivatives at the interpolation points we have a formula for the error in the derivative:

$$f'(x_j) - L_n'(x_j) = \frac{\Pi_j(x_j) f^{(n+1)}(\xi_j)}{(n+1)!}.$$

Example 1 Quadratic interpolation

$$\begin{aligned}
f(x) = f_0\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} &+ f_1\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f_2\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \\
&+ \frac{(x-x_0)(x-x_1)(x-x_2)}{3!} f^{(3)}(\xi(x))
\end{aligned}$$

$$f'(x) = f_0\frac{(2x-x_1-x_2)}{(x_0-x_1)(x_0-x_2)} + f_1\frac{(2x-x_0-x_2)}{(x_1-x_0)(x_1-x_2)} + f_2\frac{(2x-x_0-x_1)}{(x_2-x_0)(x_2-x_1)} + \text{error term}$$

$$\begin{aligned}
\therefore\ f'(x_j) = f_0\frac{(2x_j-x_1-x_2)}{(x_0-x_1)(x_0-x_2)} &+ f_1\frac{(2x_j-x_0-x_2)}{(x_1-x_0)(x_1-x_2)} + f_2\frac{(2x_j-x_0-x_1)}{(x_2-x_0)(x_2-x_1)} \\
&+ \frac{1}{3!}\prod_{\substack{i=0 \\ i\neq j}}^{2}(x_j-x_i) f^{(3)}(\xi(x_j)).
\end{aligned}$$

For the special case $x_1 = x_0 + h$, $x_2 = x_0 + 2h$

$$\begin{aligned}
f'(x_0) &= \frac{1}{h}\left[\frac{-3f_0}{2} + 2f_1 - \frac{1}{2}f_2\right] + \frac{(-h)(-2h)}{3!}f^{(3)}(\xi_0) \\
f'(x_1) &= \frac{1}{h}\left[\frac{-f_0}{2} + \frac{1}{2}f_2\right] - \frac{h^2}{6}f^{(3)}(\xi_1) \\
f'(x_2) &= \frac{1}{h}\left[\frac{f_0}{2} + 2f_1 - \frac{3}{2}f_2\right] + \frac{h^2}{3}f^{(3)}(\xi_2).
\end{aligned}$$

Example 2 Linear interpolation (equispaced)

$$\begin{aligned}
f(x) &= f_0 + \frac{\Delta f_0}{h}(x - x_0) + \frac{(x-x_0)(x-x_1)}{2}f^{(2)}(\xi(x)) \\
f'(x) &= \frac{\Delta f_0}{h} + \left[\frac{(x-x_1)}{2} + \frac{(x-x_0)}{2}\right]f^{(2)}(\xi(x)) + \frac{(x-x_0)(x-x_1)}{2}\frac{d}{dx}\left(f^{(2)}(\xi(x))\right) \\
f'(x_0) &= \frac{\Delta f_0}{h} + \frac{(x_0-x_1)}{2}f^{(2)}(\xi(x_0)) \\
f'(x_1) &= \frac{\Delta f_0}{h} + \frac{(x_1-x_0)}{2}f^{(2)}(\xi(x_1)).
\end{aligned}$$

5.2 Numerical integration

Many of the integrals that are required in practical calculation turn out to be either very hard or cannot be done using well known functions. An approximate solution is all that can be easily obtained. In this section we shall look at some simple ways to find approximations to integrals. We shall consider estimating

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

which, of course, is the area under the curve $f(x)$ between $x = a$ and $x = b$.

Method 1 The mid-point rule

Let m be the mid-point between a and b, that is $m = (a+b)/2$, then the mid-point rule approximates I by

$$I \approx M = (b-a)\,f(m)$$

and the error in this approximation can be shown to be

$$\mathrm{E}_M = I - M = \frac{(b-a)^3}{24}f^{(2)}(t_m)$$

where $f^{(p)} = \dfrac{d^p f}{dx^p}$ and t_m is some point between a and b.

We can derive this formula by approximating the function $f(x)$ by a constant that is exact at the midpoint and then integrating this approximation from a to b, see figure 1. Thus we approximate I by the area of the rectangle ABB_1A_1 namely $AB \times BB_1$ which is $(b-a)\,f(m)$.

Method 2 The trapezium rule

The trapezium rule approximates I by the area of the trapezium ABB_2A_2 indicated in figure 1. Thus

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

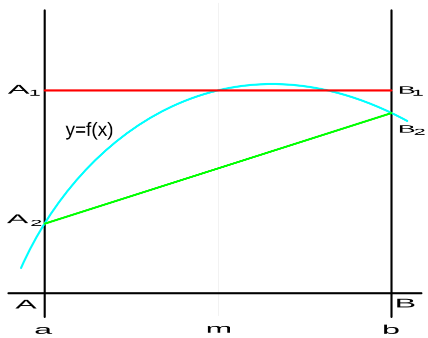

Figure 1: Mid point and trapezium rule.

The error in this approximation can be shown to be

$$E_T = I - T = -\frac{(b-a)^3}{12} f^{(2)}(t_T).$$

This rule can also be derived by approximating $f(x)$ by a linear function $L_1(x)$ which is exact at the points $x = a$ and $x = b$ and then integrating this approximation from a to b.

To show this derivation we note that

$$L_1(x) = f(a)\frac{x-b}{a-b} + f(b)\frac{x-a}{b-a}$$

and therefore

$$\begin{aligned} T &= \int_a^b L_1(x)\,dx = \frac{f(a)}{(a-b)}\int_a^b (x-b)\,dx + \frac{f(b)}{(b-a)}\int_a^b (x-a)\,dx \\ &= \frac{f(a)}{(a-b)}\left[\frac{x^2}{2} - bx\right]_a^b + \frac{f(b)}{(b-a)}\left[\frac{x^2}{2} - ax\right]_a^b = \frac{1}{2}(b-a)(f(a)+f(b)). \end{aligned}$$

Method 3 Simpson's rule

Simpson's rule provides an approximation S to I by finding a quadratic function $L_2(x)$ that approximates $f(x)$ at a, b and m and integrating this approximation from a to b. The quadratic function is

$$L_2(x) = f(a)\frac{(x-m)(x-b)}{(a-m)(a-b)} + f(m)\frac{(x-a)(x-b)}{(m-a)(m-b)} + f(b)\frac{(x-a)(x-m)}{(b-a)(b-m)}.$$

Thus, after some algebraic manipulation,

$$S = \int_a^b L_2(x)\,dx = \frac{(b-a)}{6}(f(a) + 4f(m) + f(b))$$

and it can be shown that

$$E_s = I - S = -\frac{(b-a)^5}{2880} f^{(4)}(t_s).$$

Example
We shall approximate the integral

$$I = \int_0^1 \frac{1}{1+x^2}\,dx$$

which has exact value 0.78540 by each of the above formulae. The three rules give the approximations M, T and S with errors denoted by E_M, E_T and E_S respectively.

$$\begin{aligned}
M &= \tfrac{1}{1+\left(\frac{1}{2}\right)^2} = \tfrac{4}{5} = 0.8 && E_M = -0.0146 \\
T &= \tfrac{1}{2}\left(\tfrac{1}{1+0^2} + \tfrac{1}{1+1^2}\right) = 0.75 && E_T = +0.0354 \\
S &= \tfrac{1}{6}\left(\tfrac{1}{1+0^2} + 4\tfrac{1}{1+\left(\frac{1}{2}\right)^2} + \tfrac{1}{1+1^2}\right) = 0.7833 && E_S = +0.0021
\end{aligned}$$

We can make the following comments about these results. We would expect that the more work we do, the better the result. Moreover, the formula based on the most accurate interpolation would be expected to give the best answers. Thus it is no surprise that S is the most accurate.

5.3 Improving the accuracy in numerical integration

To get a more accurate approximation we could integrate a more accurate polynomial approximation to $f(x)$ but this is seldom done. A common approach is to use the so-called composite formulae. The basic idea is to split up the range of integration into a number of smaller ranges (usually of equal length) and use either the **Trapezium rule** or **Simpson's rule** in each of the smaller intervals. For example, we get the formula $T_1 = T$ if we have just one interval, the formula T_2 in two intervals, the formula T_n in n intervals.

Thus, letting $x_0 = a$, $x_i = a + ih$, $x_n = b$ ($\therefore\ h = (b-a)/n$) and using the **trapezium rule** in each interval we obtain:

$$\begin{aligned}
\int_a^b f\,dx &= \int_{x_0}^{x_1} f\,dx + \int_{x_1}^{x_2} f\,dx + \cdots + \int_{x_{n-1}}^{x_n} f\,dx \\
&\approx \frac{h}{2}\left(f(x_0) + f(x_1)\right) + \frac{h}{2}\left(f(x_1) + f(x_2)\right) + \cdots + \frac{h}{2}\left(f(x_{n-1}) + f(x_n)\right) \\
&= \frac{h}{2}\left(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n\right) = T_n.
\end{aligned}$$

We can show that

$$E_{T_n} = I - T_n = -\frac{h^2}{12}(b-a)\,f^{(2)}(\theta_n).$$

Thus, if we compute T_n and T_{2n} we would expect the error to decrease by approximately a factor of 4.
Example Returning to the example above and using more trapeziums yields,

$$\begin{aligned}
T &= 0.75000 && E_{T_1} = 0.03540 \\
T_2 &= \tfrac{\frac{1}{2}}{2}\left(\tfrac{1}{1+0^2} + 2\tfrac{1}{1+\left(\frac{1}{2}\right)^2} + \tfrac{1}{1+1^2}\right) = 0.7750 && E_{T_2} = 0.01040 \\
T_4 &= \tfrac{\frac{1}{4}}{2}\left(\tfrac{1}{1+0^2} + 2\tfrac{1}{1+\left(\frac{1}{4}\right)^2} + 2\tfrac{1}{1+\left(\frac{2}{4}\right)^2} + 2\tfrac{1}{1+\left(\frac{3}{4}\right)^2} + \tfrac{1}{1+1^2}\right) && E_{T_4} = 0.00261 \\
&= 0.78729 \\
T_8 &= 0.78475 && E_{T_8} = 0.00065 \\
T_{16} &= 0.78524 && E_{T_{16}} = 0.00016
\end{aligned}$$

We observe that $E_{T_{2n}} \approx \frac{1}{4} E_{T_n}$.

We can do the same sort of thing with **Simpson's rule** except we define $2n+1$ points in (a, b) by $x_0 = a$, $x_i = a + ih$, $x_n = a + 2nh$, $(\therefore\ h = (b-a)/(2n))$ and apply Simpson's rule in each of the intervals (x_{2i-2}, x_{2i}) giving the composite Simpson's rule S_{2n} defined by

$$S_{2n} = \frac{h}{3}\left(f_0 + 4\sum_{odd} f_i + 2\sum_{even<2n} f_i + f_{2n}\right).$$

We can show that the error term has the form

$$E_{S_{2n}} = I - S_{2n} = -\frac{h^4}{180}(b-a)\, f^{(4)}(\sigma_{2n})$$

and we expect the error to decrease by about a factor of 16 when we halve h.

Example

$$\begin{array}{rclrcl}
S_2 & = & S = 0.78333333 & E_{S_2} & = & 0.00206483 \\
S_4 & = & 0.78539216 & E_{S_4} & = & 0.00000601 \\
S_8 & = & 0.78539813 & E_{S_8} & = & 0.00000004 \\
S_{16} & = & 0.78539816 & & & \text{exact to 8dp}
\end{array}$$

5.4 Estimating the form of the error term in numerical integration

One way of estimating the form of the error term in approximating I by the quadrature rule Q is to assume the error $I - Q$ is of the form $Cf^{(q)}(\varepsilon)$. We then find C and q by testing the rule with simple polynomials. For example, in the mid-point rule with $Q \equiv M$ we postulate

$$I - M = I - (b-a)\, f(m) = Cf^{(q)}(\varepsilon)$$

$$\begin{array}{llll}
p & \int_a^b x^p & M & \\
 & & & \\
0 & b-a & b-a & \text{exact} \\
1 & \dfrac{b^2-a^2}{2} & (b-a)\left(\dfrac{a+b}{2}\right) = \dfrac{b^2-a^2}{2} & \text{exact} \\
2 & \dfrac{b^3-a^3}{3} & (b-a)\left(\dfrac{a+b}{2}\right)^2 & \text{not exact}
\end{array}$$

The formula is exact for $p = 0$ and $p = 1$ but not exact for $p = 2$. Thus we take $q = 2$ which means that the error term $Cf^{(2)}(\xi)$ will be zero (i.e. no error) if f is a polynomial of degree less than 2. Looking at the case $p = 2$ in more detail

$$\begin{aligned}
I - M &= \frac{b^3-a^3}{3} - \frac{(b-a)(b+a)^2}{4} \\
&= \frac{(b-a)}{12}\left[4b^2 + 4ab + 4a^2 - 3b^2 - 6ab - 3a^2\right] \\
&= \frac{(b-a)}{12}\left[b^2 - 2ab + a^2\right] = \frac{(b-a)^3}{12}.
\end{aligned}$$

But $I - M = Cf^{(2)}(\xi)$ and with $f = x^2$, $f^{(2)}(\xi) = 2$ we have

$$\therefore\ 2C = \frac{(b-a)^3}{12} \quad \therefore\ C = \frac{(b-a)^3}{24}.$$

Thus, we estimate

$$E_M = \frac{(b-a)^3}{24} f^{(2)}(\xi_M).$$

It should be noted that this is only an estimate of the error not an analytic derivation of it.

We can perform the same procedure for the trapezium rule. With $Q \equiv T = \frac{(b-a)}{2}(f(a) + f(b))$ and postulating $I - T = Cf^{(q)}(\zeta)$ we get

p	$\int_a^b x^p$	T	
0	$b-a$	$b-a$	exact
1	$\frac{1}{2}(b^2-a^2)$	$\frac{b-a}{2}(a+b) = \frac{1}{2}(b^2-a^2)$	exact
2	$\frac{1}{3}(b^2-a^2)$	$\frac{b-a}{2}(a^2+b^2)$	not exact.

As above, we take $q = 2$ and note that $f^{(2)}(\xi) = 2$ when $f = x^2$. Thus we get

$$\begin{aligned} 2C &= \frac{b^3-a^3}{3} - \frac{(b-a)}{2}(b^2+a^2) \\ &= \frac{b-a}{6}(2b^2+2ab+2a^2-3b^2-3a^2) \\ &= -\frac{(b-a)^3}{6} \\ C &= -\frac{1}{12}(b-a)^3. \end{aligned}$$

There are a lot of quadrature rules

a) M, T, S as described above and similar rules based on higher order interpolation
b) Gaussian rules
c) Weighted rules, namely
$\int_a^b w(x) f(x)\, dx \approx (b-a) \sum_{i=0}^{n} \gamma_i f(x_i)$
where $w(x)$ is some weighting function.

For each quadrature rule Q we find

$$I - Q = Cf^{(q)}(\xi) \qquad a < \xi < b$$

for some C and q.