Numerical Differentiation

We also need to approximate the derivatives of functions.

One approach: Differentiate Lagrange polynomials

Suppose $x_0, x_1 \in (a,b)$ and $f \in C^2[a,b]$

Now $f(x) = P_{0,1}(x) + \frac{1}{2!}(x-x_0)(x-x_1)f''(\xi(x))$

$$= \frac{f(x_0)(x-x_1)}{x_0 - x_1} + \frac{f(x_1)(x-x_0)}{x_1 - x_0} + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x))$$

where $\xi(x) \in [a,b]$.

We can derive more general approximation formulas:

Suppose $x_0, x_1, \ldots, x_n \in (a,b)$ and $f \in C^{n+1}[a,b]$

Now $f(x) = \underbrace{\sum_{k=0}^{n} f(x_k) L_k(x)}_{P_{0,1,\ldots,n}(x)}$

$$+ \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x))$$

for some $\xi(x) \in [a,b]$

Differentiate & evaluate at $x = x_j$:

$$f'(x_j) = \sum_{k=0}^{n} f(x_k) L_k'(x_j)$$

$$+ \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{\substack{k=0 \\ k \neq j}}^{n} (x_j - x_k)$$

This is an $(n+1)$ point formula for $f'(x_j)$ since we use the $(n+1)$ values $f(x_k)$, $k = 0, \ldots, n$.

Two, three & five point formulas are the most commonly used.

Consider 3 point formulas, with x_0, x_1 & x_2.

$n=2$.

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}$$

$$\Rightarrow L_0'(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)}$$

Similarly $L_1'(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)}$

$$L_2'(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}$$

and

$$f'(x_j) = f(x_0)\frac{2x_j-x_1-x_2}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{2x_j-x_0-x_2}{(x_1-x_0)(x_1-x_2)} + f(x_2)\frac{2x_j-x_0-x_1}{(x_2-x_0)(x_2-x_1)}$$

$$+\frac{1}{6}f^{(3)}(\xi_j)\prod_{\substack{k=0\\k\neq j}}^{2}(x_j-x_k)$$

These simplify considerably when the nodes are equally spaced

$$x_1 = x_0 + h, \quad x_2 = x_0 + 2h$$

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

$$f'(x_1) = \frac{1}{h}\left[-\frac{1}{2}f(x_1-h) + \frac{1}{2}f(x_1+h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1)$$

$$f'(x_2) = \frac{1}{h}\left[\frac{1}{2}f(x_2-2h) - 2f(x_2-h) + \frac{3}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_2)$$

For convenience, replace x_1 and x_2 by x_0. This gives 3 formulas for approximating $f'(x_0)$.

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

$$f'(x_0) = \frac{1}{h}\left[-\frac{1}{2}f(x_0-h) + \frac{1}{2}f(x_0+h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1)$$

$$f'(x_0) = \frac{1}{h}\left[\frac{1}{2}f(x_0-2h) - 2f(x_0-h) + \frac{3}{2}f(x_0)\right] + \frac{h^2}{3}f^{(3)}(\xi_2)$$

Ex. Use the most appropriate three point formula to determine approximations that will complete the following table:

x	$f(x)$	$f'(x)$
1.1	9.025013	
1.2	11.02318	
1.3	13.46374	
1.4	16.44465	

1

Approximations to higher order derivatives may also be found based on function values.

Consider finding the second derivative of f:

Richardson's Extrapolation

When the error depends on some parameter such as the step size h & the dependency is predictable, we can often derive higher order accuracy from low order formulas.

To illustrate the procedure assume we have an approximation $N(h)$ to some quantity M.

Assume this approximation has an order h truncation error & that we know the expression for the first few terms of the truncation error:

$$M = N(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots$$

where the K_i's are constants, h is a positive parameter and $N(h)$ is an $O(h)$ approximation to M.

For ease of notation let

$$N_2(h) = 2N\left(\tfrac{h}{2}\right) - N(h) \qquad (***)$$

Now $M = N_2(h) - \frac{1}{2}K_2 h^2 - \frac{3}{4}K_3 h^3 - \dots$

We can repeat this calculation with $h/2$:

$$\text{Now } M = N_2\left(\tfrac{h}{2}\right) - \tfrac{1}{8}K_2 h^2 - \tfrac{3K_3}{32} h^3 - \dots \qquad (****)$$

We want to eliminate the h^2 term

Subtract four times $(****)$ from $(***)$ to give

$$3M = 4N_2\left(\tfrac{h}{2}\right) - N_2(h) + \tfrac{3}{8}K_3 h^3 + \dots$$

which gives an $O(h^3)$ formula for approximating M:

$$M = N_3(h) + \frac{K_3}{8} h^3 + \dots$$

where $N_3(h) = \frac{4}{3}N_2\left(\frac{h}{2}\right) - \frac{1}{3}N_2(h)$.

Similarly, we can derive an $O(h^4)$ approximation

$$N_4(h) = N_3\left(\tfrac{h}{2}\right) + \frac{N_3(h/2) - N_3(h)}{7}$$

$\vdots$ etc

Generally, if M can be written,

$$M = N(h) + \sum_{j=1}^{m-1} K_j h^j + O(h^m)$$

then for each $j = 2, 3, \ldots, m$ we have an $O(h^j)$ approximation of the form

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}\left(\frac{h}{2}\right) - N_{j-1}(h)}{2^{j-1} - 1}$$

In practice, higher order approximations can be systematically derived from lower order approximations:

Extrapolation can be used whenever the truncation error for a formula has the form

$$\sum_{j=1}^{m-1} K_j h^{\alpha_j} + O(h^{\alpha_m})$$

for constants K_j and

$$\alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_m.$$

Ex The following data give approximations to the integral

$$M = \int_0^{\pi} \sin x \, dx$$

$N_1(h) = 1.570769$, $N_1\left(\frac{h}{2}\right) = 1.896119$
$N_1(h/4) = 1.974232$, $N_1\left(\frac{h}{8}\right) = 1.993570$

Assuming $M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + K_4 h^8 + O(h^{10})$

Construct an extrapolation table to determine $N_4(h)$.

Soln:

Suppose $N_j(h)$ is an $O(h^{2j})$ approximation of M

then $M = N_j(h) + K_j \cdot h^{2j} + O(h^{2j+2})$ (◇)

$M = N_j\left(\frac{h}{2}\right) + K_j h^{2j}\left(\frac{1}{2}\right)^{2j} + O(h^{2j+2})$ (◇◇)

2^{2j}(◇◇) − (◇) gives

$$M = N_j\left(\frac{h}{2}\right) + \frac{N_j\left(\frac{h}{2}\right) - N_j(h)}{2^{2j}-1} + O(h^{2j+2})$$

$$\therefore N_{j+1}(h) = N_j\left(\frac{h}{2}\right) + \frac{N_j\left(\frac{h}{2}\right) - N_j(h)}{4^j-1}$$

is an $O(h^{2j+2})$ approximation of M.

Then the table becomes

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
$N_1(h) = 1.570796$			
$N_1\left(\frac{h}{2}\right) = 1.896119$	$N_2(h) = 2.004560$		
$N_1\left(\frac{h}{4}\right) = 1.974232$	$N_2\left(\frac{h}{2}\right) = 2.000270$	$N_3(h) = 1.999984$	
$N_1\left(\frac{h}{8}\right) = 1.993570$	$N_2\left(\frac{h}{4}\right) = 2.000016$	$N_3\left(h/2\right) = 1.999999$	$N_4(h)$

$N_4(h) = 1.999999$

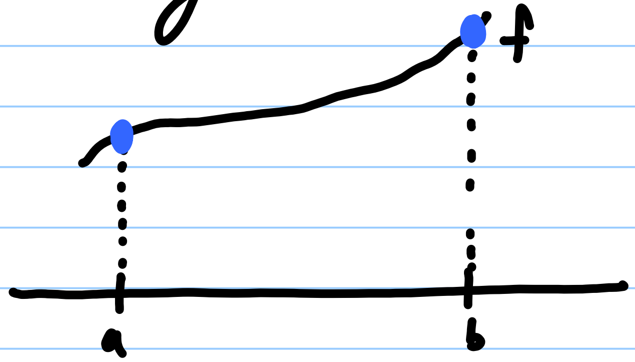
Numerical Integration

We often need to evaluate the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to obtain.

The usual strategy in developing formulas for numerical integration is similar to that for numerical differentiation. We pass a polynomial through points defined by the function and then integrate this polynomial approximation of the function. This permits us to integrate a function known only as a table of values.

We get an expression for the error by integrating the error term for our interpolating polynomial.

Suppose we use a 2 point integration formula:



Let $x_0 = a$, $x_1 = b$, $h = b - a$

The linear Lagrange polynomial passing through $(x_0, f(x_0))$ and $(x_1, f(x_1))$ is

$$P_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

& $$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} P_1(x)\,dx + \frac{1}{2}\int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\,dx$$

$$= \left. \frac{(x - x_1)^2}{2(x_0 - x_1)} f(x_0) + \frac{(x - x_0)^2}{2(x_1 - x_0)} f(x_1) \right|_{x_0}^{x_1}$$

$$+ \text{ error}$$

$$= \frac{h}{2}\left(f(x_0) + f(x_1)\right) + \text{ error}$$

Weighted Mean Value Theorem for Integrals

If $f \in C[a,b]$, the Riemann integral of g exists on $[a,b]$ and $g(x)$ does not change sign on $[a,b]$ then there exists a number c in (a,b) with

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

$$\text{error} = \frac{1}{2}\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)\, dx$$

$$= \frac{1}{2} f''(\xi)\int_{x_0}^{x_1}(x-x_0)(x-x_1)\, dx$$

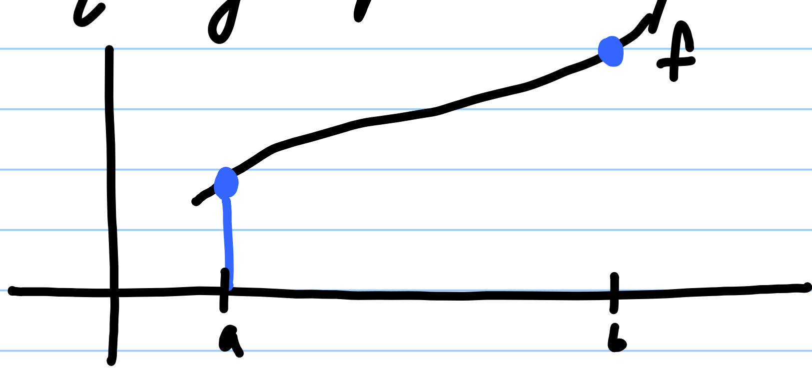
$$= \frac{1}{2} f''(\xi)\left[\frac{x^3}{3} - \frac{(x_1+x_0)}{2}x^2 + x_0 x_1 x\right]_{x_0}^{x_1}$$

$$= -\frac{h^3}{12} f''(\xi)$$

Thus $\displaystyle\int_a^b f(x)\, dx = \frac{h}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12} f''(\xi)$

The <u>trapezoid rule</u>.

We might also consider a 3 point integration formula based on equally spaced points:



If we use the usual strategy of integrating the error term for the Lagrange polynomial, then we get an $O(h^4)$ error.

A sharper estimate can be obtained using an alternative approach.

Expand f about x_1, using the third Taylor polynomial:

$$f(x) = f(x_1) + f'(x_1)(x-x_1) + \frac{f''(x_1)}{2}(x-x_1)^2 + \frac{f'''(x_1)}{6}(x-x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x-x_1)^4$$

$$\therefore \int_{x_0}^{x_2} f(x)\,dx = \Big[f(x_1)(x-x_1) + \frac{f'(x_1)}{2}(x-x_1)^2 + \frac{f''(x_1)}{6}(x-x_1)^3 + \frac{f'''(x_1)}{24}(x-x_1)^4 \Big]_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4\,dx$$

Consider $\displaystyle \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4\,dx$

$$= \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x-x_1)^4\,dx$$

$$= \frac{f^{(4)}(\xi_1)}{120}(x-x_1)^5 \Big|_{x_0}^{x_2}$$

$$= \frac{f^{(4)}(\xi_1)}{60} h^5$$

$$\therefore \int_{x_0}^{x_2} f(x)\,dx = 2h f(x_1) + \frac{h^3}{3} f''(x_1) + \frac{f^{(4)}(\xi_1)}{60} h^5$$

But from last day

$$f''(x_1) = \frac{1}{h^2}\left[f(x_0) - 2f(x_1) + f(x_2)\right] + \frac{h^2}{12} f^{(4)}(\xi_2)$$

$$\therefore \int_{x_0}^{x_2} f(x)\,dx = 2h f(x_1) + \frac{h^3}{3}\left[\frac{1}{h^2}\left(f(x_0) - 2f(x_1) + f(x_2)\right) - \frac{h^2}{12} f^{(4)}(\xi_2)\right] + \frac{f^{(4)}(\xi_1) h^5}{60}$$

$$= \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] + O(h^5)$$

Simpson's Rule.

Recall

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12} f''(\xi)$$

Trapezoid Rule

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left[f(x_0)+4f(x_1)+f(x_2)\right] - \frac{h^5}{90} f^{(4)}(\xi)$$

Simpson's Rule

What is the error for these methods if

$f(x) = x$

$f(x) = x^3$

Defn. The degree of accuracy or precision of a quadrature formula is the largest positive integer n such that the formula is exact for x^k when $k = 0, 1, \ldots, n$

	Degree of accuracy
Trapezoid Rule	
Simpson's Rule	

The Trapezoid and Simpson's Rules are examples of Newton's Cotes formulas

The $(n+1)$ point closed Newton-Cotes formula uses nodes

$$x_i = x_0 + ih, \quad i = 0, 1, \dots, n$$

where $x_0 = a$, $x_n = b$, $h = \frac{(b-a)}{n}$

Then

$$\int_a^b f(x)\,dx \approx \int_a^b P_n(x)\,dx = \int_a^b \sum_{i=0}^{n} L_i(x) f(x_i)$$

$$= \sum_{i=0}^{n} \int_a^b L_i(x)\, f(x_i)$$

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

where $a_i \equiv \int_a^b L_i(x)\,dx$

The formula is closed because the endpoints of the interval are included as nodes.

An error analysis gives

<u>Thm.</u> Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$ point closed formula with $x_0 = a$, $x_n = b$ & $h = (b-a)/n$.

If n is even & $f \in C^{n+2}[a,b]$ then there exists $\xi \in (a,b)$ with

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2 (t-1) \cdots (t-n)\,dt$$

If n is odd and $f \in C^{n+1}[a,b]$ then there exists $\xi \in (a,b)$ with

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1) \cdots (t-n)\,dt$$

Notice:

the degree of precision is $n+1$ and the error is $O(h^{n+3})$ if n is even.

If n is odd then the degree of precision is only n & the error is only $O(h^{n+2})$.

Cases

n	name	error term
1	Trapezoid Rule	$-\frac{h^3}{12} f''(\xi)$
2	Simpson's Rule	$-\frac{h^5}{90} f^{(4)}(\xi)$
3	Simpson's 3/8th Rule	$-\frac{3h^5}{80} f^{(4)}(\xi)$
4		$-\frac{8h^7}{945} f^{(6)}(\xi)$

There are also open Newton-Cotes formulas:

$$x_i = x_0 + ih \qquad i = 0, 1, \dots, n$$
$$x_0 = a + h$$
$$h = (b-a)/(n+2)$$

Then the open Newton's Cotes formulas are given by

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

where $a_i = \int_a^b L_i(x)\,dx$.

Note that $x_0 = a+h$ & $x_n = b-h$. The formulas are <u>open</u> because the nodes are all contained in the open interval (a,b).

Once again, if n is even the degree of precision is $(n+1)$ and the error is $O(h^{n+3})$

If n is odd then the degree of precision is only n and the error is only $O(h^{n+2})$.

Some examples of open Newton-Cotes formulas are

$n=0$ (Midpoint Rule)

$$\int_a^b f(x)\,dx = 2h f(x_0) + \frac{h^3}{3} f''(\xi)$$

where $\xi \in (a,b)$

$n=1$

$$\int_a^b f(x)\,dx = \frac{3h}{2}\left[f(x_0)+f(x_1)\right] + \frac{3h^3}{4} f''(\xi)$$

$n=2$

$$\int_a^b f(x)\,dx = \frac{4h}{3}\left[2f(x_0)-f(x_1)+2f(x_2)\right] + \frac{14h^5}{45} f^{(4)}(\xi)$$

$n=3$

$$\int_a^b f(x)\,dx = \frac{5h}{24}\left[11f(x_0)+f(x_1)+f(x_2)+11f(x_3)\right] + \frac{95}{144} h^5 f^{(4)}(\xi)$$

Composite Numerical Integration

Typically, we do not apply Newton-Cotes formulas to the interval $[a,b]$ directly.

If we did, then high degree formulas would be required to obtain accurate solutions.

However, we have already seen that even these high degree polynomials often give an oscillatory (& inaccurate) interpolation of high degree polynomials.

To avoid this problem, we prefer a piecewise approach to numerical integration that uses low order Newton Cotes formulas.

Ex For Simpson's Rule

Take $h = (b-a)/n$

$x_j = a + jh$

Then $$\int_a^b f(x)\,dx = \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)\,dx$$

$$= \sum_{j=1}^{n/2} \left\{ \frac{h}{3}\left[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j}) \right] - \frac{h^5}{90} f^{(4)}(\xi_j) \right\}$$

$$x_{2j-2} < \xi_j < x_{2j}$$

Taking into account that $f(x_{2j})$, $0 < j < n/2$, appears in 2 terms, this summation can be simplified somewhat

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(x_0) + 2\sum_{j=1}^{\frac{n}{2}-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right]$$

$$+ \text{ error} \rightsquigarrow \frac{-(b-a)}{180} h^4 f^{(4)}(\mu)$$

It is also important to understand the stability property of Composite Newton Cotes integration techniques

Assume $f(x_i)$ is approximated by $\tilde{f}(x_i)$:

$$f(x_i) = \tilde{f}(x_i) + e_i \qquad 0 \le i \le n$$

roundoff associated with using $\tilde{f}$ to approximate f

Then the accumulated round off error in the Composite Simpson's Rule is

$$|e(h)| = \left| \frac{h}{3}\left[e_0 + 2\sum_{j=1}^{\frac{n}{2}-1} e_{2j} + 4\sum_{j=1}^{\frac{n}{2}} e_{2j-1} + e_n \right] \right|$$

An interesting point concerning Composite Trapezoid Rule:

If $f \in C^2[a,b]$ then there exists a $\mu \in [a,b]$ s.t.

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

$$- \frac{b-a}{12} h^2 f''(\mu), \text{ where } h = \frac{b-a}{n}$$

$$x_j = a + jh$$

Thus the error for the Composite Trapezoid Rule is $O(h^2)$

In fact we can be more precise. An application of the Euler - MacLauren Summation Formula shows that for sufficiently smooth f

$$\text{error} = C_1 h^2 + C_2 h^4 + \dots + C_m h^{2m} + O(h^{2m+2})$$

where $C_k = \text{const} \times \left(f^{(2k-1)}(b) - f^{(2k-1)}(a)\right)$

Ex The numerical approximation to

$$\int_0^1 \sin^2(8\pi x)\,dx$$

by the Composite Trapezoid Rule for several values of h is given below

h	1	$1/2$	$1/4$	$1/8$	$1/16$	$1/32$	$\cdots$
Composite Trapezoid Rule	0	0	0	0	$1/2$	$1/2$	$\cdots$

Notice that we know the form of the error with Composite Trapezoid Rule. So we can combine it with Richardson Extrapolation to obtain <u>Romberg Integration</u>.

Let $R_{k,1}$ be the approximation to the integral using $m_k = 2^{k-1}$ intervals $\Rightarrow h = \frac{(b-a)}{m_k}$.

<u>ie</u>

$$R_{1,1} = \frac{h_1}{2}\left[f(a)+f(b)\right] = \frac{(b-a)}{2}\left[f(a)+f(b)\right]$$

$$R_{2,1} = \frac{h_2}{2}\left[f(a)+f(b)+2f(a+h_2)\right]$$

$$R_{3,1} = \frac{1}{2}\{R_{2,1} + h_2[f(a+h_3) + f(a+3h_3)]\}$$

$$\vdots$$

$$R_{K,1} = \frac{1}{2}\left\{R_{K-1,1} + h_{K-1}\sum_{i=1}^{2^{K-2}} f(a+(2i-1)h_K)\right\}$$

<u>Ex</u> Approx $\int_0^1 e^{-x}\,dx$

$R_{1,1} \approx 0.68394 =$

$R_{2,1} \approx 0.64523$

$R_{3,1} \approx 0.63541$

$R_{4,1} \approx 0.63294$

Next apply Richardson Extrapolation to obtain faster convergence

$$\int_a^b f(x)\,dx - R_{K,1} = c_1 h_K^2 + \sum_{i=2}^{m} c_i h_K^{2i} + O(h^{2m+2})$$

$$\int_a^b f(x)\,dx - R_{K+1,1} = \frac{c_1}{4} h_K^2 + \sum_{i=2}^{m} \frac{c_i h_K^{2i}}{4^i} + O(h^{2m+2})$$

4 times the second minus the first gives an $O(h_K^4)$ error.

We repeat the procedure to eliminate the $O(h_k^4)$ error term. Continuing we have an $O(h_k^{2j})$ approximation formula defined by

$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}.$$

Ex Use Romberg Integration to approximate

$$\int_0^1 e^{-x}\,dx \text{ to 5 significant digits}$$

Ans

	$R_{k,1}$	$R_{k,2}$	$R_{k,3}$	$R_{k,4}$	$R_{k,5}$
$R_{1,j}$	0.6839397				
$R_{2,j}$	0.6452352	0.6323337			
$R_{3,j}$	0.6354094	0.6321342	0.6321209		
$R_{4,j}$	0.6329434	0.6321214	0.6321206	0.6321206	
$R_{5,j}$	0.6323263	0.6321206	0.6321206	0.6321206	0.6321206

Adaptive Quadrature

Composite quadrature rules necessitate the use of equally spaced points

This does not take into account that some portions of the curve may have large functional variations that require more attention than other portions of the curve.

Want to approximate $\int_a^b f(x)\,dx$ to within a specified tolerance $\varepsilon > 0$.

Start by applying Simpson's Rule with a step size $h = (b-a)/2$

$$\int_a^b f(x)\,dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\mu)$$

where $S(a,b) = \frac{h}{3}\left[f(a) + 4f(a+h) + f(b)\right]$

μ is some constant $a < \mu < b$.

.

Error estimate for Simpson's Rule:

$$\text{error estimate} = \frac{1}{15}\left|S(a,b) - S\left(a, \tfrac{a+b}{2}\right) - S\left(\tfrac{a+b}{2}, b\right)\right|$$

Ex. Compute the Simpson's Rule approximations $S(a,b)$, $S\left(a, \frac{a+b}{2}\right)$, $S\left(\frac{a+b}{2}, b\right)$ for $\int_1^{1.5} x^2 \ln(x)\,dx$ & calculate the error estimate and the actual error.

Ans. $S(1, 1.5) = \frac{0.25}{3}\left[f(1) + 4f(1.25) + f(1.5)\right]$

$= 0.19224530$

$S(1, 1.25) = 0.03937243 4$

$S(1.25, 1.5) = 0.15288602$

$\therefore$ error estimate

$= \frac{1}{15}\left|S(1, 1.5) - S(1, 1.25) - S(1.25, 1.5)\right|$

$\approx 8.77 \times 10^{-7}$

actual error

$= \left|S(1, 1.25) + S(1.25, 1.5) - \text{exact}\right|$

$\approx 8.96 \times 10^{-7}$

.

Gaussian Quadrature

Thus far, we have only dealt with quadrature formulae

$$\int_a^b f(x)\,dx \approx \sum_{j=1}^{n} a_j\, f(x_j)$$

that relied on nodes that are equally spaced.

- a nice feature for composite rules because it reduces the number of function evaluations

HOWEVER, if we allow ourselves to use unequally spaced points, we can construct more accurate formulas:

n nodes & n weights
$\Longrightarrow 2n$ free parameters

We may hope to find an optimal quadrature formula which is exact for polynomials of

degree $\leq 2n-1$

We start with an integral

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

Suppose $n=2$ (2 nodes) and that we want to determine c_1, c_2, x_1, x_2 so that the integration formula

$$\int_{-1}^{1} f(x)\,dx = c_1 f(x_1) + c_2 f(x_2)$$

gives the exact result whenever $f(x)$ is a polynomial of degree 3.

ie $f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$

Since $\int_{-1}^{1} a_0 + a_1 x + a_2 x^2 + a_3 x^3 \, dx$

$$= a_0 \int_{-1}^{1} dx + a_1 \int_{-1}^{1} x\,dx + a_2 \int_{-1}^{1} x^2\,dx + a_3 \int_{-1}^{1} x^3\,dx$$

the problem is equivalent to showing the formula is exact for

$$f(x) = 1, x, x^2, x^3$$

This approach can be used to obtain the nodes and coefficients for larger n.

Sometimes, instead, we use Legendre polynomials.

The Legendre polynomials $P_0(x), P_1(x), \ldots$ are defined according to the following 2 properties

1. $P_n(x)$ is a monic polynomial of degree n.
2. $\int_{-1}^{1} P(x)\, P_n(x)\, dx = 0$ whenever $P(x)$ is a polynomial of degree less than n.

The first few Legendre polynomials are

$$P_0(x) = 1$$
$$P_1(x) = x$$
$$P_2(x) = x^2 - \frac{1}{3}$$
$$P_3(x) = x^3 - (3/5)\, x$$
$$P_4(x) = x^4 - \frac{6}{7} x^2 + 3/35$$

Some properties

- The roots of these polynomials are distinct
- The roots of these polynomials lie in $(-1, 1)$
- The P_n's are symmetrical about the origin $\Rightarrow$ the roots are symmetrical about the origin
- The roots of the n^{th} degree Legendre polynomial have the property that they are the nodes needed to produce an integral approximation formula that gives the exact results for any polynomial of degree less than $2n$.

The c_i's and the nodes are both extensively tabulated.

Note that high order Legendre polynomials are built into Maple:

```
with(orthopoly);
P(n,x);
```

Ex Approximate $\int_1^{3/2} x^2 \ln x^2 \, dx$

using Gaussian quadrature with $n = 2$.

Q. Find the constants c_0, c_1 & x_1 so that the quadrature formula

$$\int_{-1}^{0} f(x)\,dx = c_0 f(-1) + c_1 f(x_1)$$

has the highest degree of precision possible.

Ans