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

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

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

Now differentiate:

$$f'(x) = \frac{f(x_1)-f(x_0)}{x_1 - x_0} + D_x\left[\frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x))\right]$$

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

Typically, we want derivative values <u>at the nodes</u>. Then the last error term is zero...

For example at $x = x_0$

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

Typically we set $x_1 = x_0 + h$, then

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2} f''(\xi)$$

This is known as a <u>forward difference formula</u> if $h > 0$ and a <u>backward difference formula</u> if $h < 0$.

We can derive more general approximation formulas:

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

Now
$$f(x) = \underbrace{\sum_{k=0}^{n} f(x_k) L_k(x)}_{P_{0,1,\dots,n}(x)} + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x))$$

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

Differentiate and 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 and five point formulas are the most commonly used formulas.

Consider 3 point formulas with x_0, x_1 and 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

$$f'(x_j) = f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right]$$

$$+ f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right]$$

$$+ f(x_2)\left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}\right]$$

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

These simplify considerably when the nodes are equally spaced

$$x_1 = x_0 + h$$
$$x_2 = x_0 + 2h$$

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

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

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

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

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

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

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

<u>Ex</u> 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	

ANS. $f'(1.1) \approx \frac{1}{2(0.1)}\left[-3f(1.1)+4f(1.2)-f(1.3)\right] = 17.769705$

$f'(1.2) \approx \frac{1}{2(0.1)}\left[f(1.3)-f(1.1)\right] = 22.193635$

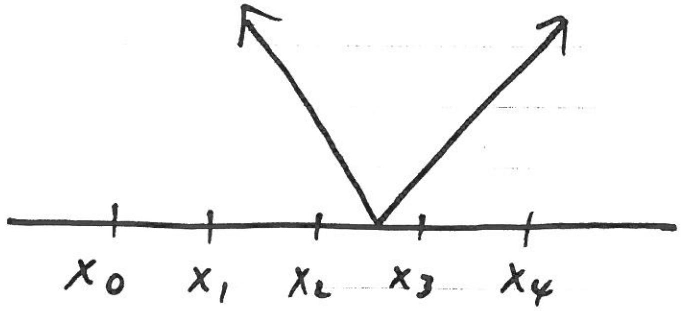
$f'(1.3) \approx \frac{1}{2(0.1)}\left[f(1.4)-f(1.2)\right] = 27.107350$

$f'(1.4) \approx \frac{1}{2(0.1)}\left[f(1.2)-4f(1.3)+f(1.4)\right] = 32.510850$

Notice that at the end points we must use one sided differences.

In the interior, we used centered differencing. Centered differences often have a smaller error constant when f is smooth & they require fewer operations to compute.

Which points would you ~~difference~~ use to compute the first ~~difference~~ derivative approximation at x_1 & x_2?



x_1 :

x_2 :

One sided and centered five point formulas can also be derived in a similar manner.

$$f'(x_0) = \frac{1}{12h}\left[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\right] + \frac{h^4}{30} f^{(5)}(\xi)$$

(centered differencing)

$$f'(x_0) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)\right] + \frac{h^4}{5} f^{(5)}(\xi)$$

(One sided differencing — Left endpoint approximations are found using $h>0$ and right endpoint approximations are found using $h<0$)

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

Consider finding the second ~~derivation~~ derivative of f:

$$f(x_0+h) = f(x_0) + f'(x_0)h + \tfrac{1}{2} f''(x_0)h^2 + \tfrac{1}{6}f'''(x_0)h^3 + \tfrac{1}{24}f^{(4)}(\xi_1)h^4$$

$$f(x_0-h) = f(x_0) - f'(x_0)h + \tfrac{1}{2} f''(x_0)h^2 - \tfrac{1}{6}f'''(x_0)h^3 + \tfrac{1}{24}f^{(4)}(\xi_{-1})h^4$$

where $x_0-h < \xi_{-1} < x_0 < \xi_1 < x_0+h$

Summing:

$$f(x_0+h) + f(x_0-h) = 2f(x_0) + f''(x_0)h^2 + \frac{h^4}{24}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]$$

We assume $f^{(4)}$ is continuous on $[x_0-h,\ x_0+h]$.

Since $\frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]$ is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_{-1})$

the intermediate value theorem implies that there is a number ξ between ξ_1 and ξ_2 with $f^{(4)}(\xi) = \frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]$

$$\therefore\ f(x_0+h) + f(x_0-h) = 2f(x_0) + f''(x_0)h^2 + \frac{h^4}{24} f^{(4)}(\xi)$$

$$\Longrightarrow\ f''(x_0) = \frac{1}{h^2}\left[f(x_0-h) - 2f(x_0) + f(x_0+h)\right] - \frac{h^2}{24} f^{(4)}(\xi)$$

Notice that all the differentiation formulas divide by some power of h. Division by small numbers tends to exaggerate roundoff error, but this is an effect that cannot be entirely avoided in numerical differentiation.

Thus we do not want to take h to be too small because then the roundoff errors will dominate the calculation.

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 and that we know the expression for the first few terms of the truncation error,

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

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

We can repeat the calculation with a parameter $\left(\frac{h}{2}\right)$:

$$M = N\left(\frac{h}{2}\right) + K_1\left(\frac{h}{2}\right) + K_2\left(\frac{h^2}{4}\right) + K_3\left(\frac{h^3}{8}\right) \quad (**)$$

Now

We want to obtain a higher order method by using some combination of these results.

Subtract (*) from twice (**) gives

$$M = \left[2N\left(\frac{h}{2}\right) - N(h)\right] + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots$$

which is an $O(h^2)$ approximation formula for M.

For ease of notation let $N_2(h) = 2N(h/2) - N(h)$.

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

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

Now $$M = N_2\left(\frac{h}{2}\right) - \frac{1}{8}K_2 h^2 - \frac{3K_3}{32} h^3 - \cdots \quad (****)$$

We want to eliminate the h^2 term.

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

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

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

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

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

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

and an $O(h^5)$ approximation

$$N_5(h) = N_4\left(\tfrac{h}{2}\right) + \frac{N_4(h/2) - N_4(h)}{15}.$$

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

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

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

$$\begin{array}{cccc}
O(h) & O(h^2) & O(h^3) & O(h^4) \\
N_1(h) & & & \\
N_1(h/2) & N_2(h) & & \\
N_1(h/4) & N_2(h/2) & N_3(h) & \\
N_1(h/8) & N_2(h/4) & N_3(h/2) & N_4(h)
\end{array}$$

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

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

$$N_1(h) = 1.570796, \quad N_1(h/2) = 1.896119$$
$$N_1(h/4) = 1.974232, \quad N_1(h/8) = 1.993570$$

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.

$$M = N_1(h) + K_1 h^2 + O(h^4) \quad (*)$$
$$M = N_1\left(\tfrac{h}{2}\right) + \left(\tfrac{1}{2}\right)^2 K_1 h^2 + O(h^4) \quad (**)$$

$2^2(**) - (*)$ gives $(4-1)M = N_1\left(\tfrac{h}{2}\right)(4-1) + N_1\left(\tfrac{h}{2}\right) - N_1(h) + O(h^4)$

$$\Rightarrow \quad M = N_1\left(\tfrac{h}{2}\right) + \frac{N_1(h/2) - N_1(h)}{4-1} + O(h^4)$$

Thus $N_2(h) \equiv \dfrac{4N_1(h/2) - N_1(h)}{3}$ is an $O(h^4)$ approximation of M.

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

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

$2^{2j}(\diamond\diamond) - (\diamond)$ gives

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

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

Then the table becomes

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
$N_1(h) = 1.570796$			
$N_1(h/2) = 1.896119$	$N_2(h) = 2.004560$		
$N_1(h/4) = 1.974232$	$N_2(h/2) = 2.000270$	$N_3(h) = 1.999984$	
$N_1(h/8) = 1.993570$	$N_2(h/4) = 2.000016$	$N_3(h/2) = 1.999999$	$N_4(h) = 1.99999$

So extrapolation can produce high order approximations with minimal computational cost.

It is important to be aware that as higher order extrapolations are used, more roundoff error will be generated. We may also increase the likelihood of numerical instabilities in some situations.

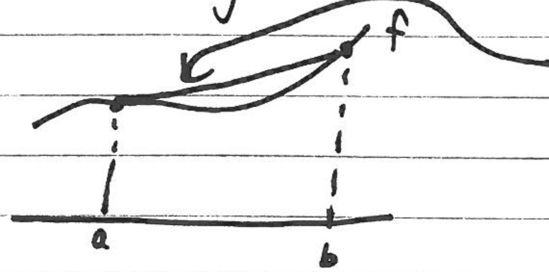
Numerical Integration.

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:



interpolating polynomial based on 2 points

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

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

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

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

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

To evaluate the error we will need the

Weighted Mean Value Thm for Integrals.

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

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

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

$$= \frac{1}{2} f''(\underbrace{\xi}_{\text{some number in } [x_0,x_1]}) \int_{x_0}^{x_1} (x-x_0)(x-x_1)\,dx$$

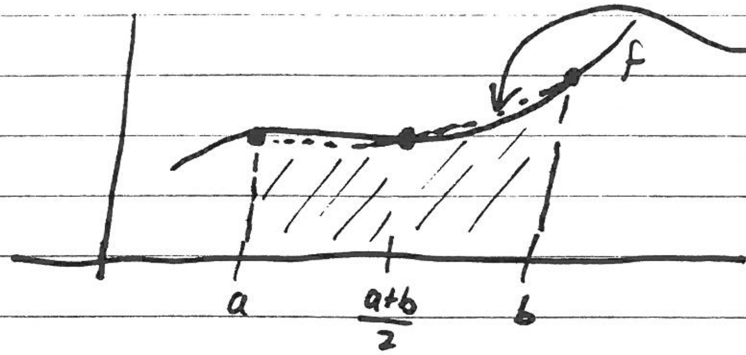
$$= \frac{1}{2} f''(\xi)\left[x^3/3 - \frac{(x_1+x_0)}{2}x^2 + x_0x_1x\right]_{x_0}^{x_1}$$

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

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

This is known as the trapezoid rule since the integral is approximated by the area of a trapezoid.

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



interpolating polynomial based on 3 equally spaced nodes

$x_0 = a$

$x_1 = a + h$ $\qquad h = \frac{b-a}{2}$

$x_2 = b$

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:

$$f(x) = f(x_1) + f'(x_1)(x-x_1) + \frac{f''(x_1)}{2}(x-x_1)^2$$

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

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

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

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

$$= \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x-x_1)^4\,dx$$ by the weighted mean value Thm for some $\xi_1 \in (a,b)$

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

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

$\therefore$ $$\int_0^{x_2} f(x)\,dx = 2h f(x_1) + \frac{h^3}{3}f''(x_1) + \frac{f^{(4)}}{60}(\xi_1)h^5$$

But from last day,

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

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

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

This integration rule is known as Simpson's Rule:

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] \underbrace{- \frac{h^5}{90} f^{(4)}(\xi)}_{\text{will be shown as part of assignment 4.}}$$

Recall from last day:

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

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 Simpson's Rule if

$f(x) = x$

$f(x) = x^3$

<u>Defn</u>: 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 <u>Newton-Cotes formulas.</u>

The $(n+1)$ point <u>closed</u> Newton - Cotes formula uses nodes $x_i = x_0 + ih$ for $i = 0, 1, \dots, n$ where

$$x_0 = a$$
$$x_n = b$$
$$h = (b-a)/n.$$

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 of the Newton-Cotes formulas gives an interesting result:

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

If n is even and $f \in C^{n+2}[a,b]$ 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 that 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 and 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 Three Eigths Rule	$-\frac{3h^5}{80} f^{(4)}(\xi)$
4		$-\frac{8h^7}{945} f^{(6)}(\xi)$

There are also <u>open</u> Newton-Cotes formulas

Here $\quad x_i = x_0 + ih \qquad i = 0, 1, \ldots, n$

$$x_0 = a + h$$
$$h = (b-a)/(n+2)$$

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

Note that $x_0 = a + h$ and $x_n = b - h$. 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).

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

$n=1$
$$\int_a^b f(x)\,dx = \frac{3h}{2}\left[f(x_0)+f(x_1)\right] + \frac{3h^3}{4} f''(\xi) \quad \text{where } \xi \in (a,b)$$

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

$n=3$
$$\int_a^b f(x)\,dx = \frac{5h}{24}\left[11f(x_0)+f(x_1)+f(x_2)+11f(x_3)\right] + \frac{95}{144} h^5 f^{(4)}(\xi)$$

Composite Numerical Integration

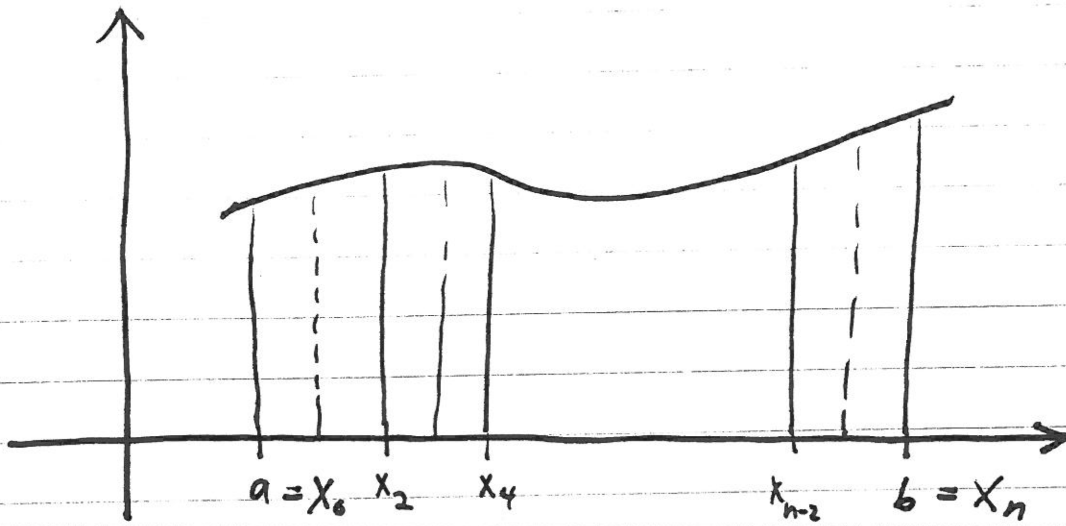
Typically, we do not apply Newton-Cotes formulas to the interval $[a,b]$ directly.

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 (and 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.



We divide the interval into an even number of subintervals.

Simpson's rule is applied on each consecutive pair of sub intervals.

Take $h = (b-a)/n$
$x_j = a + jh$

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

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

where $x_{2j-2} < \xi_j < x_{2j}$
and $f \in C^4[a,b]$.

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

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

where $\text{error} = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j)$

To simplify this error we will need the

Extreme Value Theorem:

If $f \in C[a,b]$, then $c_1, c_2 \in [a,b]$ exist with

$f(c_1) \leq f(x) \leq f(c_2)$ for each $x \in [a,b]$

$$\text{error} = -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j)$$

If $f \in C^4[a,b]$, the EVT implies that $f^{(4)}$ assumes its maximum and minimum in $[a,b]$

$$\therefore \quad \min_{x\in[a,b]} f^{(4)}(x) \le f^{(4)}(\xi_j) \le \max_{x\in[a,b]} f^{(4)}(x)$$

$1 \le j \le n/2$

Sum over all j:

$$\frac{n}{2}\min_{x\in[a,b]} f^{(4)}(x) \le \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \frac{n}{2}\max_{x\in[a,b]} f^{(4)}(x)$$

$$\Rightarrow \quad \min_{x\in[a,b]} f^{(4)}(x) \le \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \max_{x\in[a,b]} f^{(4)}(x)$$

By the IVT, there is a $\mu \in (a,b)$ s.t.

$$f^{(4)}(\mu) = \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j)$$

$$\therefore \quad \text{error} = -\frac{hn}{180} h^4 f^{(4)}(\mu)$$

$$= -\frac{(b-a)}{180} h^4 f^{(4)}(\mu).$$

The subdivision approach can be applied to any of the low order formulas. For example:

<u>Thm</u>: Let $f \in C^2[a,b]$
$h = (b-a)/n$
$x_j = a + jh \qquad 0 \le j \le n$

There exists a $\mu \in (a,b)$ for which the Composite Trapezoid Rule for n subintervals can be written with its error term as

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

$$- \frac{(b-a)}{12} h^2 f''(\mu)$$

Q. Show that the error for Composite Simpson's Rule can be approximated by

$$-\frac{h^4}{180}\left[f'''(b)-f'''(a)\right].$$

Ans.

$$\text{error} = -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j)$$

$$= -\frac{h^4}{180}\sum_{j=1}^{n/2} f^{(4)}(\xi_j)\,2h$$

$$\doteq -\frac{h^4}{180}\int_a^b f^{(4)}(x)\,dx$$

$$= -\frac{h^4}{180}\left[f'''(b)-f'''(a)\right]$$

(Recall that the Riemann integral of the function f on the interval $[a,b]$ is the following limit provided it exists

$$\int_a^b f(x)\,dx = \lim_{\max \Delta x_i \to 0} \sum_{i=1}^{n} f(z_i)\,\Delta x_i$$

where the numbers $x_0, x_1, \ldots, x_n$ satisfy $a = x_0 \le x_1 \le \cdots \le x_n = b$ and where $\Delta x_i = x_i - x_{i-1}$ and z_i is arbitrarily chosen in the interval $[x_{i-1}, x_i]$ for $1 \le i \le n$.

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

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

$$f(x_i) = \tilde{f}(x_i) + \underbrace{e_i}_{\text{roundoff associated with using } \tilde{f} \text{ to approximate } f} \qquad 0 \le i \le n$$

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

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

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

If the roundoff errors are uniformly bounded by ε then

$$|e(h)| \le \frac{h}{3} \left[\varepsilon + 2\left(\frac{n}{2}-1\right)\varepsilon + 4\frac{n}{2}\varepsilon + \varepsilon \right]$$

$$= \frac{h}{3} 3n\varepsilon$$

$$= nh\varepsilon$$

$$= (b-a)\varepsilon$$

which is independent of $h \Rightarrow$ the procedure is stable as $h \to 0$.