Lecture 5: Numerical Integration

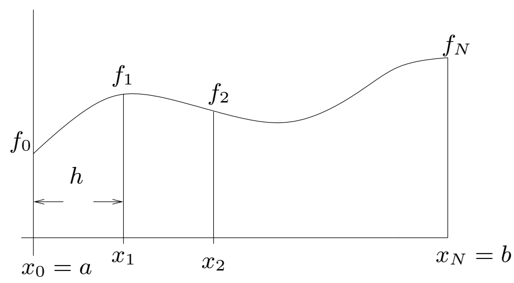
(*Compiled 16 August 2017*)

In this lecture we introduce techniques for numerical integration, which are primarily based on integrating interpolating polynomials and which lead to the so-called Newton-Cotes Integration Formulae. We derive the classic integration schemes such as the trapezium rule and Simpson's rule and give their error estimates. We demonstrate how these error estimates can be used to obtain improved estimates of the integral via a process called Richardson Extrapolation. In fact, repeated extrapolation using the trapezium rule yields Simpson's rule and all the higher order Newton-Cotes Formulae

Key Concepts: Numerical Integration, Newton-Cotes Formulae, Trapezium Rule, Simpson's Rule, Richardson Extrapolation.

5 Numerical Integration - Newton-Cotes Formulae

5.1 Integration derived from integrating polynomial interpolants



Basic Idea: Integrate polynomial interpolants to approximate integrals.

$$f(x) = p_N(x) + \frac{f^{(N+1)}(\xi)}{(N+1)!}\prod_{j=0}^{N}(x-x_j) \qquad \xi \in (x_0, x_N) \qquad p_N(x) = \sum_{k=0}^{N} f_k \ell_k(x)$$

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_a^b p_N(x)\,dx + \frac{f^{(N+1)}(\xi)}{(N+1)!}\int_a^b \prod_{j=0}^{N}(x-x_j)\,dx \\ &= \sum_{k=0}^{N} f_k \int_a^b \ell_k(x)\,dx + \frac{f^{(N+1)}(\xi)}{(N+1)!}\int_a^b \prod_{j=0}^{N}(x-x_j)\,dx \\ &= \sum_{k=0}^{N} f_k w_k + \frac{f^{(N+1)}(\xi)}{(N+1)!}\int_a^b \prod_{j=0}^{N}(x-x_j)\,dx\end{aligned}$$

Outline:

- Closed Formulae Trapezium Rule → Adaptive Integration → Richardson Extrapolation and Simpson's Rule
- Singular integrals and open formulae → Midpoint Rule → Subtracting out the singularity
- Gauss-Legendre quadrature

The Trapezium Rule:

$$f_p = E^p f_0 = (1+\Delta)^p f_0 \simeq (1+p\Delta) f_0$$

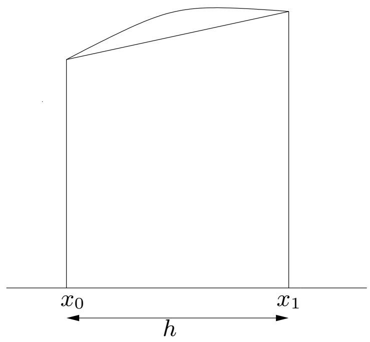
$$x = x_0 + ph, \quad dx = h dp$$

$$\int_{x_0}^{x_1} f(x)\,dx \simeq h \int_0^1 (f_0 + p\Delta f_0)\,dp$$

$$= h\left[f_0 p + \frac{p^2}{2}\Delta f_0\right]_0^1$$

$$= h\left[f_0 + \frac{1}{2}(f_1 - f_0)\right]$$

$$= \frac{h}{2}[f_0 + f_1] \qquad \text{Trapezoidal Rule}$$



Error Term:

$$f(x) = p_1(x) + \frac{f^{(2)}(\xi)}{2!}(x-x_0)(x-x_1)$$

$$x = x_0 + ph$$

$$x - x_0 = ph$$

$$x - x_1 = x_0 + ph - x_1 = (p-1)h$$

$$\therefore \int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}\,[f_0+f_1] + \frac{f^{(2)}(\xi)}{2}\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx$$

$$= \frac{h}{2}[f_0+f_1] + \frac{f^{(2)}(\xi)}{2}\,h\int_0^1 (ph)(p-1)h\,dp$$

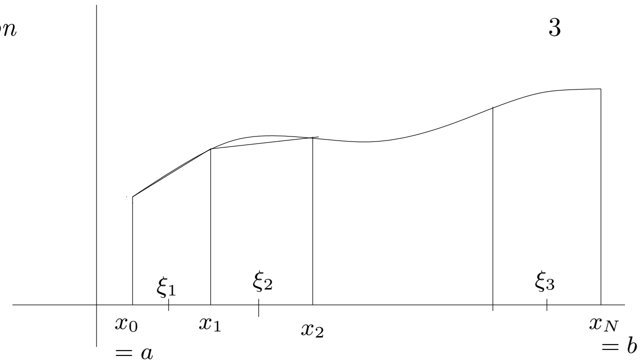
$$= \frac{h}{2}[f_0+f_1] + \frac{f^{(2)}(\xi)}{2}\,h^3\int_0^1 p^2 - pdp$$

$$= \frac{h}{2}[f_0+f_1] + \frac{f^{(2)}(\xi)}{2}\,h^3\left[\frac{p^3}{3} - \frac{p^2}{2}\right]_0^1$$

$$\frac{1}{3} - \frac{1}{2} = \frac{2-3}{6} = -\frac{1}{6}$$

$$\boxed{\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}[f_0+f_1] - \frac{f^{(2)}(\xi)h^3}{12}}$$

Composite Rule: Assume a uniform mesh



$$\int_a^b f(x)\,dx = \frac{h}{2}(f_0+f_1) + \frac{h}{2}(f_1+f_2) + \cdots + \frac{h}{2}(f_{N-1}+f_N)$$

$$-\frac{h^2}{12}\left\{h\sum_{k=1}^{N} f^{(2)}(\xi_k)\right\}$$

$$\simeq \frac{h}{2}\Big[f_0+2f_1+\cdots+2f_{N-1}+f_N\Big] - \frac{h^2}{12}\Big\{f'(b)-f'(a)\Big\} + \frac{h^4}{720}\Big(f^{(3)}(b)-f^{(3)}(a)\Big) - \cdots$$

$$\boxed{\int_a^b f(x)\,dx = \frac{h}{2}\Big[f_0+2f_1+\cdots+2f_{N-1}+f_N\Big] - \frac{h^2}{12}(b-a)f''(\xi) \quad \xi\in(a,b) \text{ by MV Theorem.}}$$

Note:

(1) Trapezoidal Rule is excellent for approximating periodic functions

Eg. If $f(x)$ is periodic on $[a,b]$ i.e. $f(a)=f(b)$ then

$$\int_a^b f(x)\,dx = h\sum_{k=0}^{N-1} f_k$$

Recall the DFT $\displaystyle \frac{1}{2\pi}\int_0^{2\pi} e^{-ikx} f(x)\,dx \simeq \frac{1}{2\pi}\left(\frac{2\pi}{N}\right)\sum_{j=0}^{N-1} e^{-ik\left(\frac{2\pi}{N}\right)j} f_j = \hat{f}_k$

(2) Accuracy for periodic functions:

If $\quad f'(a)=f'(b)$ then $\displaystyle\int_a^b f(x)\,dx = h\sum_{j=0}^{N-1} f_j + O(h^4)$

If $\quad f^{(3)}(a)=f^{(3)}(b)$ then $\displaystyle\int_a^b f(x)\,dx = h\sum_{j=0}^{N-1} f_j + O(h^6)$

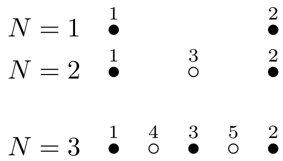
$\vdots$

If $\quad f^{(2k+1)}(a)=f^{(2k+1)}(b) \qquad k=0,1,\ldots,M$ then $\displaystyle\int_a^b f(x)\,dx = h\sum_{j=0}^{N-1} f_j + O\Big(h^{2(M+1)}\Big)$

This is where the spectral accuracy comes from.

(3) **Adaptive Integration**:

Idea: Recursively refine the sampling of the integrand until the difference between successive approximate integrals is less than some tolerance.



$$2 + 2^{2-2} + 2^{3-2} + \cdots + 2^{k-2}$$

$$\begin{aligned} 2 + 1 + 2 + \cdots + 2^{k-2} &= 2 + \frac{(1-2^{k-1})}{(1-2)} \\ &= 2 + (2^{k-1} - 1) \\ &= 1 + 2^{k-1} \end{aligned}$$

$$I_1 = \frac{h}{2}(f_1 + f_2) = \frac{(b-a)}{2}(f_1 + f_2)$$

$$i = 2^{N-2} = 1 \qquad h_2 = (b-a)/i = (b-a)$$

$$x = a + \frac{h_2}{2} : h_2 : b = \left[\frac{(b-a)}{2}\right].$$

$$I_2 = \frac{1}{2}\left\{I_1 + h_2 f_3\right\} = \frac{\left(\frac{b-a}{2}\right)}{2}(f_1 + f_2) + \frac{(b-a)}{2} f_3$$

$$= \frac{(b-a)}{4}\left[f_1 + 2f_3 + f_2\right]$$

$$i = 2^{3-2} = 2 \quad h_3 = (b-a)/2$$

$$x = a + \frac{h_3}{2} : h_3 : b = \left[\left(\frac{b-a}{4}\right), 3\left(\frac{b-a}{4}\right)\right]$$

$$I_3 = \frac{1}{2}\left\{I_2 + h_3(f_4 + f_5)\right\}$$

$$= \frac{1}{2}\left\{\frac{(b-a)}{4}[f_1 + 2f_3 + f_2] + \frac{(b-a)}{2}(f_4 + f_5)\right\}$$

$$= \frac{\left\{\frac{(b-a)}{4}\right\}}{2}\left[f_1 + 2f_3 + 2f_4 + 2f_5 + f_2\right]$$

In general :

$$I_k = \frac{1}{2}\left\{I_{k-1} + \frac{(b-a)}{2^{k-2}} \sum_{j=j_k+1}^{j_k+2^{k-2}} f_j\right\}$$

$$j_k = 1 + 2^{k-2}$$

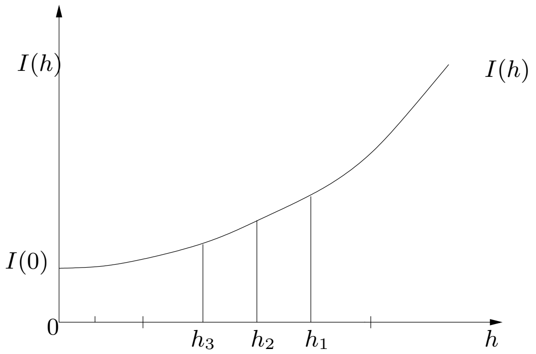
Trapezoidal Approximation:

Example:

N	$\int_0^1 \sqrt{x}\, dx$	$\int_0^1 \sin \pi x\, dx$	$\int_0^1 \sin^2 \pi x\, dx$
2	0.60355339	0.50000000	0.00000000
4	0.64328305	0.60355339	0.50000000
8	0.65813022	0.62841744	0.50000000
16	0.66358120	0.63457315	0.50000000
32	0.66555894	0.63610836	0.50000000
64	0.66627081	0.63649193	0.50000000
⋮			
Exact	$0.66666666\dot{6}$	0.63661977	0.50000000
	$O(h^?)$	$O(h^2)$	$O(h^m)$

Richardson Extrapolation:

Exploiting the error estimate to get an improved approximation:



Because we have an error estimate for the Trapezium rule of the form:

$$I(h) = I(0) + c_2 h^2 + c_4 h^4 \qquad I(4h) = I(0) + c_2 16h^2 + c_4 256h^4$$
$$I(2h) = I(0) + c_2 4h^2 + c_4 16h^4$$

eliminate the c and get an improved estimate:

$$4I(h) - I(2h) = 3I(0) - 12c_4 h^4$$
$$\therefore \quad \frac{4I(h) - I(2h)}{3} = I(0) - 4c_4 h^4$$

Example:

$$I = \int_0^1 \sin \pi x \, dx$$
$$I(1/4) = 0.60355339059327$$
$$I(1/8) = 0.62841743651573$$
$$\therefore \quad \frac{4I(1/8) - I(1/4)}{3} = 0.6370545 \approx 0.63661977$$

We can continue with this process using the recursion

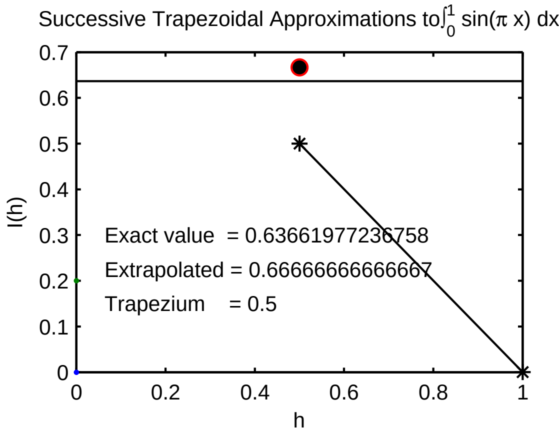
$$a_s^{(1)} = I(h_s) \qquad s = 1, \ldots, k$$
$$a_s^{(m)} = a_{s+1}^{(m-1)} + \frac{\left(a_{s+1}^{(m-1)} - a_s^{(m-1)}\right)}{\left(h_s / h_{s+m-1}\right)^{\gamma} - 1} \qquad \begin{array}{l} s = 1, \ldots, k-m+1 \\ m = 2, \ldots, k \end{array}$$

and where expansion for the error is of the form

$$I(h) = I(0) + \sum_{k=1}^{N} C_{\gamma k} (h^{\gamma})^k$$

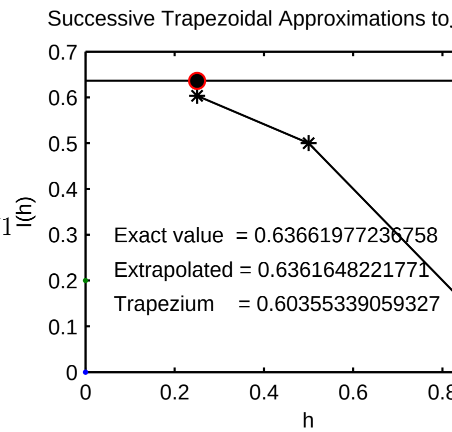
Note: Richardson extrapolation combined with adaptive integration is known as Romberg integration.

Repeated Richard Extrapolation:



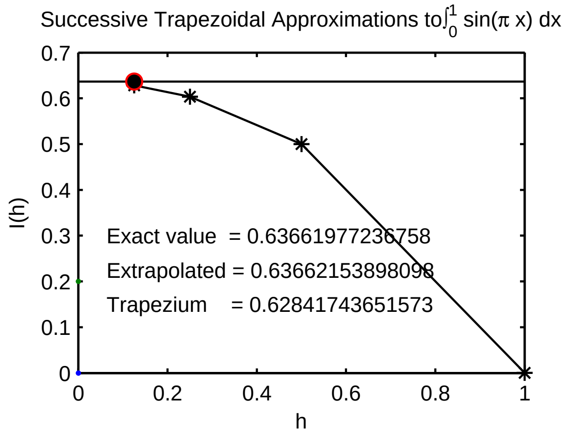
Extrapolation 1:

h	$a^{(1)} = I(h)$	$a^{(2)}$
1.000000000000000	0.000000000000000	0.666666666666667
0.500000000000000	0.500000000000000	



Extrapolation 2:

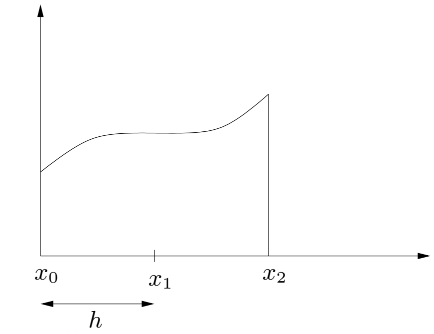
h	$a^{(1)} = I(h)$	$a^{(2)}$	$a^{(2)}$
1.000000000000000	0.000000000000000	0.666666666666667	0.6361648221771
0.500000000000000	0.500000000000000	0.638071187457698	
0.250000000000000	0.603553390593274		



Extrapolation 3:

h	$a^{(1)} = I(h)$	$a^{(2)}$	$a^{(2)}$	$a^{(3)}$
1.000000000000000	0.000000000000000	0.666666666666667	0.636164822177100	0.636621538980979
0.500000000000000	0.500000000000000	0.638071187457698	0.636614402780918	
0.250000000000000	0.603553390593274	0.636705451823217		
0.125000000000000	0.628417436515731			

Simpson's Rule:



$$p = \frac{x - x_0}{h}$$
$$x = x_0 + ph$$
$$dx = h dp$$

Recall

$$\begin{aligned} E^p f_0 &= (1+\Delta)^p f_0 \\ &= \left(1 + p\Delta + \frac{p(p-1)}{2!}\Delta^2 + \dots\right) f_0 \\ E^p f_0 &\approx \left(1 + p\Delta + \frac{p(p-1)}{2}\Delta^2\right) f_0 \qquad \text{for a polynomial of degree 2.} \\ \int_{x_0}^{x_2} f(x)\, dx &= h \int_0^2 \left(f_0 + p\Delta f_0 + \frac{1}{2}(p^2 - p)\Delta^2 f_0\right) dp \\ &= h\left\{p f_0 + \frac{p^2}{2}\Delta f_0 + \frac{1}{2}\left(\frac{p^3}{3} - \frac{p^2}{2}\right)\Delta^2 f_0\right\}_0^2 \\ &= h\left\{2f_0 + 2(f_1 - f_0) + \frac{1}{2}\left(\frac{8}{3} - 2\right)(f_2 - 2f_1 + f_0)\right\} \\ &= h\left\{2f_1 + \frac{1}{3}f_2 - \frac{2f_1}{3} + \frac{1}{3}f_0\right\} \end{aligned}$$

$$\boxed{\int_{x_0}^{x_2} f(x)\, dx = \frac{h}{3}\left\{f_0 + 4f_1 + f_2\right\}} \qquad \text{Simpson's Rule (Requires 2 intervals).}$$

Error involved:

$$\int_{x_0}^{x_2} f(x)\, dx = \int_{x_0}^{x_2} P_2(x)\, dx + \frac{f^{(3)}(\xi)}{3!}\int_{x_0}^{x_2} (x - x_0)(x - x_1)(x - x_2)\, dx$$

$$\chi = x - x_1 \quad x = x_1 + \chi$$

$$\int_{x_0}^{x_2} (x - x_0)(x - x_1)(x - x_2)\, dx = \int_{-h}^{h} (\chi + h)\chi(\chi - h) d\chi = \int_{-h}^{h} \chi^3 - h^2\chi\, d\chi = 0.$$

$$\therefore \int_{x_0}^{x_2} f(x)\, dx = \frac{h}{3}\{f_0 + 4f_1 + f_2\} + \int_{x_0}^{x_2} f[x_0, x_1, x_2, x](x - x_0)(x - x_1)(x - x_2)\, dx$$

Now

$$f[x_0,x_1,x_2,x]-f[x_0,x_1,x_2,x_3]=(x-x_3)f[x_0,x_1,x_2,x_3,x]$$

$$\therefore \int_{x_0}^{x_2} f[x_0,x_1,x_2,x](x-x_0)(x-x_1)(x-x_3)dx = \int_{x_0}^{x_2} f[x_0,x_1,x_2,x_3](x-x_0)(x-x_1)(x-x_2)\,dx$$

$$+\int_{x_0}^{x_2} f[x_0,x_1,x_2,x_3,x](x-x_0)(x-x_1)(x-x_2)(x-x_3)\,dx$$

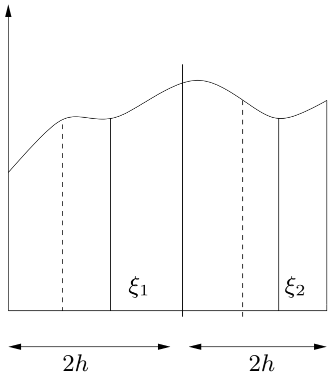
$$\int_{x_0}^{x_2} f(x)dx = S + \frac{f^{(4)}(\xi)}{4!}\int_{x_0}^{x_2}(x-x_0)(x-x_1)(x-x_2)(x-x_3)\,dx \qquad \text{choose } x_3=x_1$$

$$\int_{x_0}^{x_2}(x-x_0)(x-x_1)^2(x-x_2)\,dx = \int_{-h}^{h}\left(\chi^2-h^2\right)\chi^2 d\chi = \frac{2h^5}{5}-\frac{2h^5}{3} = h^5\frac{6-10}{15} = -\frac{4h^5}{15}$$

$$\boxed{\therefore \int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left\{f_0+4f_1+f_2\right\} - \frac{f^{(4)}(\xi)}{90}h^5}$$

Composite Rule:

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+\ldots+4f(x_{N-1})+f(x_N)\right] - \frac{h^5}{90}\sum_{k=1}^{N/2} f^{(4)}(\xi_k)$$



$$\int_a^b f(x)dx = S - \frac{h^4}{180}(2h)\sum_{k=1}^{N/2} f^{(4)}(\xi_k)$$

$$= S - \frac{h^4}{180}\left(f^{(3)}(b)-f^{(3)}(a)\right)$$

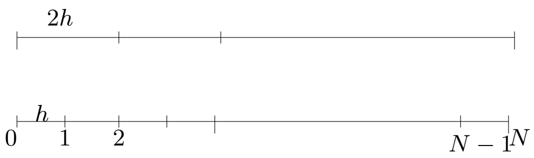
$$= S - \frac{h^4}{180}(b-a)f^{(4)}(\xi)$$

$$2h\sum_{k=1}^{N/2} f^{(4)}(\xi_k) \approx \int_a^b f^{(4)}(x)\,dx$$

$$= f^{(3)}(b)-f^{(3)}(a)$$

Richard Extrapolation leads to higher order Newton-Cotes formulae: Neat interpretation of the first extrapolation formula for the trapezium rule:

$$I(0) = \frac{4}{3}I(h) - \frac{1}{3}I(2h) + O(h^4)$$



$$\begin{aligned} I(0) &= \frac{4}{3} \cdot \frac{h}{2}\Big\{ f_0 + 2f_1 + \cdots + 2f_{N-1} + f_N \Big\} - \frac{1}{3}\frac{\cancel{2}h}{\cancel{2}}\Big\{ f_0 + 2f_2 + \cdots + 2f_{N-2} + f_N \Big\} \\ &= \frac{h}{3}\Big\{ f_0 + 4f_1 + 2f_2 + \cdots + 2f_{N-2} + 4f_{N-1} + f_N \Big\} \qquad \text{just Simpson's Rule.} \end{aligned}$$

Note: If we repeat this process we obtain the higher order Newton-Cotes Formulae.

Closed Newton-Cotes Formulae:

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12}\,f^{(2)}(\xi) \qquad \text{Trapezium rule} \qquad \xi \in (x_0, x_1)$$

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{h^5}{90}\,f^{(4)}(\xi) \qquad \text{Simpson's rule} \qquad \xi \in (x_0, x_2)$$

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3h^5}{80}\,f^{(4)}(\xi) \qquad \xi \in (x_0, x_3)$$

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) - \frac{8h^7}{945}\,f^{(6)}(\xi) \qquad \xi \in (x_1, x_4)$$