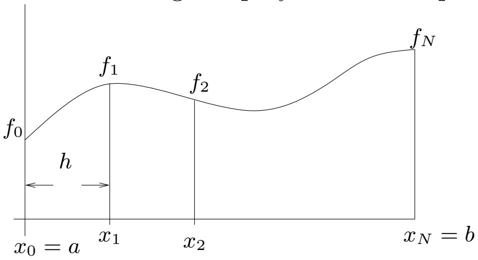
Numerical Integration

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

  Simpson's Rule

- Singular integrals and open formulae

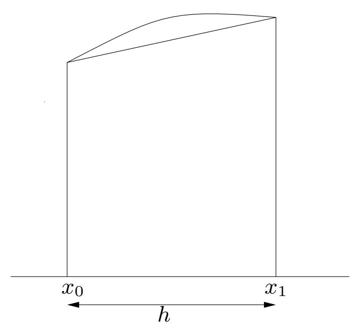
  – Midpoint Rule

  – Subtracting out the singularity

- Gauss-Legendre quadrature

The Trapezium Rule:

$$
\begin{aligned}
f_p = E^p f_0 &= (1+\Delta)^p f_0 \simeq (1+p\Delta) f_0 \\
x &= x_0 + ph, \quad dx = hdp \\
\int_{x_0}^{x_1} f(x)\,dx &\simeq h\int_0^1 (f_0 + p\Delta f_0)\,dp \\
&= h\left[f_0 p + \frac{p^2}{2}\Delta f_0\right]_0^1 \\
&= h\left[f_0 + \frac{1}{2}(f_1 - f_0)\right] \\
&= \frac{h}{2}[f_0 + f_1] \qquad \textsc{Trapezoidal Rule}
\end{aligned}
$$



Error Term:

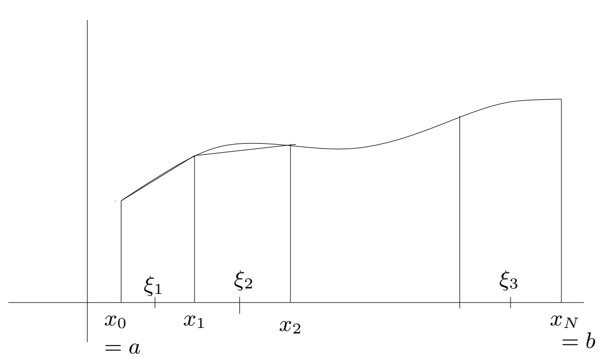
$$
\begin{aligned}
f(x) &= p_1(x) + \frac{f^{(2)}(\xi)}{2!}(x-x_0)(x-x_1) \\
\therefore \int_{x_0}^{x_1} f(x)\,dx &= \frac{h}{2}\,[f_0+f_1] + \frac{f^{(2)}(\xi)}{2}\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx \\
&= \frac{h}{2}[f_0+f_1] + \frac{f^{(2)}(\xi)}{2}\,h\int_0^1 (ph)(p-1)h\;dp \\
&= \frac{h}{2}[f_0+f_1] + \frac{f^{(2)}(\xi)}{2}\,h^3\int_0^1 p^2 - pdp \\
&= \frac{h}{2}[f_0+f_1] + \frac{f^{(2)}(\xi)}{2}\,h^3\left[\frac{p^3}{3} - \frac{p^2}{2}\right]_0^1
\end{aligned}
$$

$$
\begin{aligned}
x &= x_0 + ph \\
x - x_0 &= ph \\
x - x_1 &= x_0 + ph - x_1 = (p-1)h
\end{aligned}
$$

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

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

Composite Rule: Assume a uniform mesh



$$
\begin{aligned}
\int_a^b f(x)\,dx &= \frac{h}{2}\left(f_0+f_1\right)+\frac{h}{2}\left(f_1+f_2\right)+\cdots+\frac{h}{2}\left(f_{N-1}+f_N\right) \\
&\quad -\frac{h^2}{12}\left\{h\sum_{k=1}^{N} f^{(2)}(\xi_k)\right\} \\
&\simeq \frac{h}{2}\Big[f_0+2f_1+\cdots+2f_{N-1}+f_N\Big]-\frac{h^2}{12}\Big\{f'(b)-f'(a)\Big\}+\frac{h^4}{720}\Big(f^{(3)}(b)-f^{(3)}(a)\Big)-\cdots
\end{aligned}
$$

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

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:

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

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

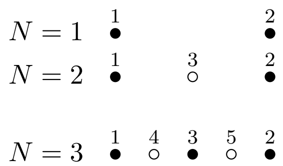
   $$\vdots$$

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

   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.



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

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

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

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

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

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

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

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

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

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

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

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

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
	$O(h^?)$	$O(h^2)$	$O(h^m)$