Chapter 10. Numerical Integration.

Error function $\operatorname{erf}(x) \equiv \dfrac{2}{\sqrt{\pi}} \underbrace{\int_0^x e^{-t^2}\,dt}_{\text{cannot be evaluated analytically}}$
important in probability and statistics.

$\Downarrow$ numerical integration.

Formulas used in Chapter 10 are often called quadrature formulas: Latin word "quadratus" (i.e. "square") is used as ancient mathematicians were trying to find the area under the curve by finding a square w/ approximately the same area.

§ 10.1 Newton – Cotes Formulas.

$\hookrightarrow$ Roger Cotes (1682 - 1716)

To find $\int_a^b f(x)\,dx$, replace $f(x)$ by its polynomial interpolant $p(x)$: $\int_a^b f(x)\,dx \approx \int_a^b p(x)\,dx =$

$$= \underbrace{\sum_{i=0}^{n} f(x_i) \int_a^b \left(\prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j} \right) dx}_{\text{Newton-Cotes formula}}$$

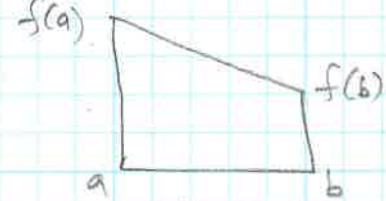
(using Lagrange form for p, w/ equally spaced nodes)

Let $n=1 \Rightarrow$ the trapezoid rule!

$$f(x) \approx p_1(x) = f(a)\frac{x-b}{a-b} + f(b)\frac{x-a}{b-a} \qquad \begin{pmatrix} x_0 = a, \\ x_1 = b \end{pmatrix}$$

$$\Rightarrow \int_a^b f(x)\,dx \approx \frac{f(a)}{a-b}\int_a^b (x-b)\,dx + \frac{f(b)}{b-a}\int_a^b (x-a)\,dx =$$

$$= \frac{f(a)}{a-b}\frac{(x-b)^2}{2}\Big|_a^b + \frac{f(b)}{b-a}\frac{(x-a)^2}{2}\Big|_a^b = \underbrace{\frac{b-a}{2}\left[f(a)+f(b)\right]}_{\text{area of the trapezoid}}$$



What about the error?

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

$$= \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi_x)\left(\prod_{i=0}^{n}(x-x_i)\right)dx$$

<u>for $n=1$</u>: $\int_a^b f(x)\,dx - \int_a^b p_1(x)\,dx = \frac{1}{2}\int_a^b f''(\xi_x)(x-b)(x-a)\,dx$ — ξ_x depends on x

$$= \frac{1}{2}f''(\eta)\int_a^b (x-a)(x-b)\,dx \qquad \eta \in [a,b]$$

MVT for integrals

$$= -\frac{(b-a)^3}{12}f''(\eta)$$

$$\int_a^b f(x)g(x)\,dx = f(c)\int_a^b g(x)\,dx, \quad c\in[a,b]$$

if $g(x)$ does not change sign in $[a,b]$

Here $\underbrace{(x-b)}_{<0}\underbrace{(x-a)}_{>0} < 0 \quad \forall x \in [a,b]$

<u>Example:</u> $\int_0^2 e^{-x^2}dx \approx \frac{2-0}{2}\left[e^{-4}+e^{0}\right] = 1+e^{-4} \approx 1.0183$

w/ the error $= -\frac{(2-0)^3}{12}f''(\eta) = -\frac{2}{3}f''(\eta)$, $\eta\in[0,2]$

$$f'(x) = -2xe^{-x^2}$$

$$f''(x) = (4x^2-2)e^{-x^2} \Rightarrow \max_{[0,2]}|f''(x)| = |f''(0)| = 2$$

$$\Rightarrow |\text{error}| \le 4/3$$

for $n=2$: $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$ $\Rightarrow$

$$\underbrace{p_2(x)}_{\deg 2} = f(a)\frac{\left(x-\frac{a+b}{2}\right)(x-b)}{\left(a-\frac{a+b}{2}\right)(a-b)} + f\left(\frac{a+b}{2}\right)\frac{(x-a)(x-b)}{\left(\frac{a+b}{2}-a\right)\left(\frac{a+b}{2}-b\right)}$$

$$+ f(b)\frac{(x-a)\left(x-\frac{a+b}{2}\right)}{(b-a)\left(b-\frac{a+b}{2}\right)} \Rightarrow \underbrace{\int_a^b f(x)\,dx \approx \int_a^b p_2(x)\,dx}$$

Instead: we can use the method of undetermined coefficients, $\Leftarrow$ messy to integrate

i.e.: $$\int_a^b f(x)\,dx \approx A_1 f(a) + A_2 f\left(\frac{a+b}{2}\right) + A_3 f(b)$$

This formula must be exact for all polynomials of deg 2 or less (the formula must integrate each of the quadratic terms in $p_2(x)$ correctly). For example,

$$\text{If } \varphi_1(x) = \frac{\left(x-\frac{a+b}{2}\right)(x-b)}{\left(a-\frac{a+b}{2}\right)(a-b)} \Rightarrow \int_a^b \varphi_1(x)\,dx$$

$$= A_1 \underbrace{\varphi_1(a)}_{=1} + A_2 \underbrace{\varphi_1\left(\frac{a+b}{2}\right)}_{=0} + A_3 \underbrace{\varphi_1(b)}_{=0} \Rightarrow A_1 = \int_a^b \varphi_1(x)\,dx.$$

If we pick polynomials $1, x, x^2$, then

$$\int_a^b 1\,dx = b-a = A_1\cdot 1 + A_2\cdot 1 + A_3\cdot 1 \Rightarrow A_1 + A_2 + A_3 = b-a$$

$$\int_a^b x\,dx = \frac{b^2-a^2}{2} = A_1 a + A_2\frac{a+b}{2} + A_3 b$$

$$\int_a^b x^2\,dx = \frac{b^3-a^3}{2} = A_1 a^2 + A_2\left(\frac{a+b}{2}\right)^2 + A_3 b^2$$

$\Rightarrow$ solving for A_1, A_2, A_3 gives:

$$A_1 = A_3 = \frac{b-a}{6},\quad A_2 = \frac{4(b-a)}{6} \quad \text{and}$$

$$\underbrace{\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]}_{\text{Simpson's rule.}}$$

(area under quadratic curve that interpolates f at a, $\frac{a+b}{2}$, b)

Example : $\int_0^2 e^{-x^2}\,dx \approx \frac{1}{3}\left[e^0 + 4e^{-1} + e^{-4}\right] \approx 0.8299$

Error? Read p.p. 230-231 (Taylor's thm again) to understand the error in Simpson's rule:

$$\frac{1}{2880}(b-a)^5 f^{(4)}(\xi), \quad \xi \in [a,b]$$

Thus, the error for this example is

$$\left| \frac{2^5}{2880} f^{(4)}(\xi) \right|_{\xi \in [0,2]} \le \frac{2^5}{2880} \cdot 12 = 0.1333.$$

(knowing that $|f^{(4)}(x)| \le 12$ for $x \in [0,2]$)