Chapter 10. Numerical Integration.

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

cannot be evaluated analytically $\Downarrow$ 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) $\rightarrow$ English mathematician

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

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

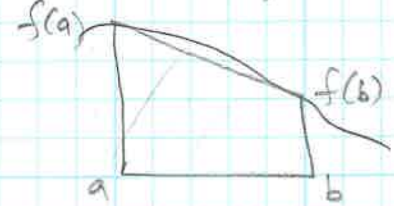
(using Lagrange form for p, w/ equally spaced nodes)

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

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

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

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



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>; $\displaystyle\int_a^b f(x)\,dx - \int_a^b p_1(x)\,dx = \frac{1}{2}\int_a^b f''(\xi_x)(x-b)(x-a)\,dx$ ↳ depends on x

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

MVT for integrals (applied to f'')

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

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

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

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

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

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

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

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 ← messy to integrate
of undetermined coefficients,

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,

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

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

(Similar for A_2, A_3)

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:

$A_1 = A_3 = \frac{b-a}{6}$, $A_2 = \frac{4(b-a)}{6}$ 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 : $\displaystyle\int_0^2 e^{-x^2}\,dx \approx \frac{1}{3}\left[e^0 + 4e^{-1} + e^{-4}\right] \approx 0.8299$

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

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

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