PHYS 177
winter 2019

<u>lecture 5 : error estimation</u>

learning goals
- estimate error in a numerical integral
- search for and use standard integration methods

to estimate integration error, start with a function expansion around 2 points

$$f(x) = \begin{cases} f(x_{i-1}) + (x-x_{i-1})f'(x_{i-1}) + (x-x_{i-1})^2 f''(x_{i-1}) + \dots \\ f(x_i) + (x-x_i)f'(x_i) + (x-x_i)^2 f''(x_i) + \dots \end{cases}$$

then we can integrate

$$\int_{x_{i-1}}^{x_i} dx f(x) = \begin{cases} \int_0^{\Delta x} du \left[f(x_{i-1}) + u f'(x_{i-1}) + u^2 f'(x_{i-1}) + \dots \right] \\ \int_{-\Delta x}^{0} dv \left[f(x_i) + v f'(x_i) + v^2 f''(x_i) + \dots \right] \end{cases}$$

averaging these gives

note the minus sign

$$\int_{x_{i-1}}^{x_i} dx f(x) = \frac{1}{2} \Big\{ \Delta x \left[f(x_{i-1}) + f(x_i) \right] + \frac{1}{2}\Delta x^2 \left[f'(x_{i-1}) - f'(x_i) \right] + \frac{1}{6}\Delta x^3 \left[f''(x_{i-1}) + f''(x_i) \right] + \dots \Big\}$$

we can then write the whole integral as a sum over discrete intervals

$$\begin{aligned} \int_a^b dx f(x) &= \sum_i \int_{x_{i-1}}^{x_i} dx f(x) \\ &= \sum_i \Delta x \frac{f(x_{i-1}) + f(x_i)}{2} \quad \leftarrow \text{trapezoid} \\ &+ \sum_i \frac{\Delta x^2}{4} \left[f'(x_{i-1}) - f'(x_i) \right] \longrightarrow = \frac{\Delta x^2}{4} \left[f'(a) - f'(b) \right] \\ &+ \sum_i \frac{\Delta x^3}{6} \frac{f''(x_{i-1}) + f''(x_i)}{2} \quad \leftarrow \propto \text{trapezoidal integral of } f'' \\ &+ \mathcal{O}(\Delta x^4) \end{aligned}$$

integrating the trapezoidal sum for f'' and canceling terms, we get error on the trapezoidal integral

$$\epsilon = \frac{\Delta x^2}{12} \left[f'(a) - f'(b) \right] + \mathcal{O}(\Delta x^4)$$

note: for other integration rules, need a different expansion, see <u>Newman</u>

for Simpson's rule, $\epsilon = \frac{\Delta x^4}{90} \left[f'''(a) - f'''(b) \right] + \mathcal{O}(\Delta x^6)$

theoretical error is great, but what if we have no analytical expression for f'?

start by performing integral w/ N_1 steps, record answer I_1

integrate again with $N_2 = 2N_1$ steps, so $\Delta x_1 = 2\Delta x_2$

then write

some constant

$$I = I_1 + c\Delta x_1^2 = I_1 + 4c\Delta x_2^2 = I_2 + c\Delta x_2^2$$

$$I_2 - I_1 = 3c\Delta x_2^2, \text{ so } \epsilon_2 = c\Delta x_2^2 = \tfrac{1}{3}(I_2 - I_1)$$

aside

how important is rounding error?

each numerical computation includes a rounding error that is well-approximated by a normal (Gaussian) random variable w/ mean 0 and standard deviation

$$\sigma = Cx, \text{ w/ } C \sim 10^{-16}$$

w/out going into detail, sum of N normal variables w/ std σ has typical size $\propto \sqrt{N}\sigma$

but trapezoidal rule multiplies by $\Delta x \propto 1/N$, so cumulative error drops like $1/\sqrt{N}$!

*notebook example w/ scipy package