Numerical Integration (Quadrature)

- *NRiC* Chapter 4.
- Already seen Monte Carlo integration.
- Can cast problem as a differential equation (DE):

$$I = \int_a^b f(x)\, dx$$

is equivalent to solving for $I \equiv y(b)$ the DE $dy/dx = f(x)$ with the boundary condition (BC) $y(a) = 0$.

  - Will learn about ODE solution methods next class.

Trapezoidal & Simpson's Rule

- Have abscissas $x_i = x_0 + ih$, $i = 0, 1, ..., N + 1$.
- A function $f(x)$ has known values $f(x_i) = f_i$.
- Want to integrate $f(x)$ between endpoints a & b.
- Trapezoidal rule (2-point closed formula):

$$\int_{x_1}^{x_2} f(x)\,dx = h\left[\frac{1}{2}f_1 + \frac{1}{2}f_2\right] + O\left(h^3 f^{(2)}\right)$$

- Simpson's rule (3-point closed formula):

$$\int_{x_1}^{x_3} f(x)\,dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3\right] + O\left(h^5 f^{(4)}\right)$$

Extended Trapezoidal Rule

- If we apply the Trapezoidal rule *N* -1 times and add the results, we get:

$$\int_{x_1}^{x_N} f(x)\,dx = h\left[\frac{1}{2}f_1 + f_2 + f_3 + \quad + f_{N-1} + \frac{1}{2}f_N\right] + O\left(h^3 f^{(2)}\right)$$

- Big advantage is it builds on previous work:
  - Coarsest step: average *f* at endpoints *a* and *b*.
  - Next refinement: add value at midpoint to average.
  - Next: add values at ¼ and ¾ points.
  - And so on. This is implemented as `trapzd()` in *NRiC*.

More Sophistication

- Usually don't know *N* in advance, so iterate to a desired accuracy: `qtrap()`.
- Higher-order method by cleverly adding refinements to cancel error terms: `qsimp()`.
- Generalization to order 2*k* (*Richardson's deferred approach to the limit*): `qromb()`.
- For improper integrals, generally need *open formulae* (not evaluated at endpoints).
- For multi-*D*, use nested 1-*D* techniques.