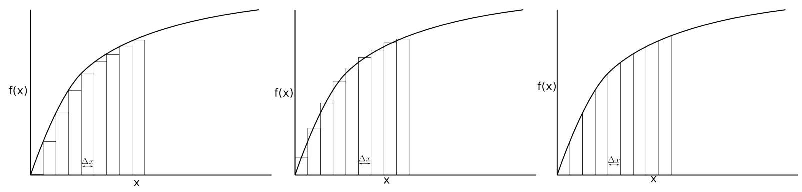

Figure 1: Numerical integration methods. The first method is a poor method, the midpoint method (second) and trapazoid rule (third) are both useful schemes.

Numerical Integration

- Integration: area or volume defined by a region.
- Numerical integration divides problem into slivers, and adds together the area of each sliver.

Numerical integration:

- to evaluate complex problems (no analytic solution)
- generally applicable integrator

Many examples where numerical integration is applicable

- special functions (error function $[\frac{2}{\sqrt{\pi}} \int_0^x e^{-x^2} dx]$,exponential integral $[\int_x^\infty \frac{e^{-t}}{t} dt]$)
- flow through a tube (vel is function of r) $Q = \int v(r) 2\pi r dr$
- estimate size of ore deposit
- estimate area of watershed

There are many numerical integration schemes.

Newton-Cotes

- use a simple polynomial
- fit function in piecewise fashion
- rectangle rules-zeroth-order polynomial used:

$$\int_a^b f(x)dx \approx \sum_i f(x_i)\Delta x$$

- the height of the rectangle is estimated by evaluating the function at some point in the interval Δx

Truncation Error

$$f(x+\Delta x) = f(x) + f(x)' \frac{\Delta x}{1} + f(x)'' \frac{\Delta x^2}{2} + f(x)''' \frac{\Delta x^3}{6} \ldots$$
$$\int (f(x+\Delta x) - f(x)) = f(x)\frac{\Delta x}{1} + f(x)' \frac{\Delta x^2}{2} + f(x)'' \frac{\Delta x^3}{6} \ldots$$

- exact integral in blue,
- rectangle rule in purple
- truncation error for a single slice in black.

Summing the error over all the slices:

$$e \approx \sum_n f(x)' \frac{\Delta x^2}{2}$$

$$e \approx f(x)'_{ave} \frac{x_{total}}{\Delta x} \frac{\Delta x^2}{2}$$

- Rectangle rule is first order accurate.
- Using similar method proves trapezoid rule is second order accurate.

Trapezoid Rule

The trapezoid rule results from a first-order polynomial:

$$\int_a^b f(x)dx \approx \sum_i \frac{f(x) + f(x+\Delta x)}{2} \Delta x$$

Simpson's Rule

Simpson's rule results when a second-order polynomial is used to approximate the function.

$$f(x) = Ax^2 + Bx + C$$
$$f(\Delta x) = A\Delta x^2 + B\Delta x + C$$
$$f(0) = A \cdot 0^2 + B \cdot 0 + C$$
$$f(-\Delta x) = A\Delta x^2 - B\Delta x + C$$

Combining the last three equations to solve for A and B

$$A = \frac{f(\Delta x) - 2f(x) + f(-\Delta x)}{2\Delta x^2}$$
$$B = \frac{f(\Delta x) - f(-\Delta x)}{2\Delta x}$$
$$C = f(x)$$

Integrating the polynomial from Δx to $-\Delta x$ and substituting A and C into equation:

$$\int_{-\Delta x}^{+\Delta x} f(x) = \left(\frac{A\Delta x^3}{3} + \frac{B\Delta x^2}{2} + C\Delta x\right) - \left(\frac{-A\Delta x^3}{3} + \frac{B\Delta x^2}{2} + -C\Delta x\right)$$
$$= 2\frac{A\Delta x^3}{3} + 2C\Delta x$$
$$= 2\frac{\frac{f(\Delta x)-2f(0)+f(-\Delta x)}{2\Delta x^2}\Delta x^3}{3} + 2f(0)\Delta x$$
$$= \frac{\Delta x}{3}(f(\Delta x) - 2f(0) + f(-\Delta x) + 6f(0))$$
$$\int_{-\Delta x}^{+\Delta x} f(x) = \frac{\Delta x}{3}(f(x-\Delta x) + 4 \cdot f(x) + f(x+\Delta x))$$

Despite the improvements associated with Simpson's Rule, it may be better to use the midpoint method with smaller increments.

Richardson Extrapolation

Richardson extrapolation utilizes an estimate of the truncation error to refine the calculated area.
The truncation error for the trapezoid rule can be estimated using the Taylor Series:

$$\int_x^{x+\Delta x} f(x) = g(x+\Delta x) - g(x)$$
$$g(x+\Delta x) - g(x) = \frac{\Delta x}{1!} f(x) + \frac{\Delta x^2}{2!} f'(x) + \frac{\Delta x^3}{3!} f(x)'' + \ldots$$

Here, $g(x+\Delta x)$-$g(x)$ is the exact integral. Note that each term in the Taylor Series has been integrated once.
Applying the Taylor Series to the first derivative:

$$g(x+\Delta x) - g(x) = \frac{\Delta x}{1!} f(x) + \frac{\Delta x^2}{2!} f'(x) + \ldots$$

Substitute Taylor series approx. for $f^{'}(x) = \frac{f(x+\Delta x)-f(x)}{\Delta x} + \frac{\Delta x}{2!}f^{''}(x) + \ldots$:

$$g(x+\Delta x) - g(x) = \frac{\Delta x}{1!}f(x) + \frac{\Delta x^2}{2!}\left(\frac{f(x+\Delta x)-f(x)}{\Delta x} + \frac{\Delta x}{2!}f^{''}(x) + \ldots\right)$$
$$+\frac{\Delta x^3}{3!}f^{''}(x)\ldots$$
$$g(x+\Delta x) - g(x) = \Delta x\left(\frac{f(x+\Delta x)+f(x)}{2}\right) - \frac{1}{12}\Delta x^3 f(x)^{''}\ldots$$

The error relative to step size and for total integral:

$$E \approx -\frac{1}{12}\Delta x^3 f(x)^{''}$$
$$E_{total} \approx \Delta x^2 x_{total} f(x)^{''}_{ave}$$

Applying this to the trapazoid rule:

$$I(\Delta x) = \int_x^{x+\Delta x} f(x) = \Delta x\frac{f(x+\Delta x)+f(x)}{2} + S_T \cdot \Delta x^2$$

by estimating the integral using two step sizes (eg. Δx and $\frac{\Delta x}{2}$), S_T can be calculated and the error in the numerical integration can be reduced

$$I \approx \Delta x\frac{f(x+\Delta x)+f(x)}{2} + S_T \cdot \Delta x^2$$
$$I \approx \frac{\Delta x}{2}\frac{f(x)+f(x+\frac{\Delta x}{2})}{2} + \frac{\Delta x}{2}\frac{f(x+\frac{\Delta x}{2})+f(x+\Delta x)}{2} + S_T \cdot \left(\frac{\Delta x}{2}\right)^2$$

Using $I(\Delta x)$ to indicate the trapezoid rule estimate using a spacing of Δx:

$$I \approx I(\Delta x) + S_T \cdot \Delta x^2$$
$$I \approx I(\frac{\Delta x}{2}) + S_T \cdot \left(\frac{\Delta x}{2}\right)^2$$
$$I(\Delta x) + S_T \cdot \Delta x^2 \approx I(\frac{\Delta x}{2}) + S_T \cdot \left(\frac{\Delta x}{2}\right)^2$$
$$S_T \approx \frac{I(\Delta x) - I(\frac{\Delta x}{2})}{\left(\frac{\Delta x}{2}\right)^2 - \Delta x^2}$$

Romberg Integration is based on this method, applying is sequentially to reduce error

Integrating to ∞

Strategies:

- break into two integrals where function can be simplified and evaluated to infinity
- use finite limits and increase size until change is no longer significant

Breaking into two regions

$$\int_0^{\infty} \frac{1}{e^{-x}+e^{x}} \approx \int_0^{10} \frac{1}{e^{-x}+e^{x}} + \int_{10}^{\infty} \frac{1}{e^{x}}$$
$$\int_0^{\infty} \frac{1}{e^{-x}+e^{x}} \approx \int_0^{10} \frac{1}{e^{-x}+e^{x}} + -e^{-x}\,|_{10}^{\infty}$$