Gaussian Quadrature

Newton - Coates rule is of the form

$$\int_a^b f(x)\,dx \approx \sum w_j f(x_j)$$

where x_j's are equidistant

this is not always optimal

* Choose $n+1$ points in $[a,b]$ & $n+1$ weights, so $2n+2$ unknowns

on $[-1,1]$, lets look at $n=1$ (2 points)

find w_0, w_1, x_0, x_1

$$\int_{-1}^{1} f(x)\,dx \approx w_0 f(x_0) + w_1 f(x_1)$$

<u>Goal</u>: want exactness for polynomials of degree 3

$$f(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3$$

$$\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} c_0 + c_1 x + c_2 x^2 + c_3 x^3\,dx$$

$$= w_0 (c_0 + c_1 x_0 + c_2 x_0^2 + c_3 x_0^3)$$
$$+ w_1 (c_0 + c_1 x_1 + c_1 x_1^2 + c_3 x_1^3)$$

Rewrite as

$$c_0 \left(w_0 + w_1 - \int_{-1}^{1} 1 \, dx \right) + c_1 \left(w_0 x_0 + w_1 x_1 - \int_{-1}^{1} x \, dx \right)$$
$$+ c_2 \left(w_0 x_0^2 + w_1 x_1^2 - \int_{-1}^{1} x^2 \, dx \right)$$
$$+ c_3 \left(w_0 x_0^3 + w_1 x_1^3 - \int_{-1}^{1} x^3 \, dx \right) = 0$$

$$\Rightarrow w_0 + w_1 = \int_{-1}^{1} 1 \, dx = 2$$
$$w_0 x_0 + w_1 x_1 = \int_{-1}^{1} x \, dx = 0$$
$$w_0 x_0^2 + w_1 x_1^2 = \int_{-1}^{1} x^2 \, dx = \frac{2}{3}$$
$$w_0 x_0^3 + w_1 x_1^3 = \int_{-1}^{1} x^3 \, dx = 0$$

$$w_0 = 1 \quad w_1 = 1 \quad x_0 = -\frac{\sqrt{3}}{3} \quad x_1 = \frac{\sqrt{3}}{3}$$

$$\boxed{\int_{-1}^{1} f(x) \, dx = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)}$$

For any $[a, b]$

$$t = a_0 + a_1 x_1 \qquad t(a) = -1 \qquad t(b) = 1$$

$$[a, b] \longrightarrow [-1, 1]$$

$$a_0 = -\frac{b+a}{b-a} \qquad a_1 = \frac{2}{b-a}$$

$x = \frac{b-a}{2} t + \frac{b+a}{2}$ $\quad dx = \frac{b-a}{2} dt$

$$\int_a^b f(x)dx = \underbrace{\int_{-1}^{1} f\left(\frac{(b-a)t + b+a}{2}\right) \frac{b-a}{2} dt}_{\text{use standard formula}}$$

Generalization

- for $[-1,1]$ $\Rightarrow$ for 1 point we should use $x=0$

  - for 2 points $\left(\pm \frac{1}{\sqrt{3}}\right)$

Thm (Gauss)

If $q(x)$ is a polynomial of degree $n+1$

so $\int_a^b x^k q(x) dx = 0 \quad k=0,\dots,n$

& let $x_0, x_1, \dots, x_n$ be the zeros of $q(x)$ in $[a,b]$

$$\Rightarrow \int_a^b f(x)dx \approx \sum_{i=0}^{n} A_i f(x_i)$$

$$A_i = \int_a^b l_i(x)dx \qquad i=0,\dots,n$$

l_i : Lagrange basis polynomials on $x_0, \dots x_n$

Higher dimensions

① $\int_{\Omega} f(x,y)\,dx\,dy \quad \Omega = [a,b] \times [c,d]$

② $\int_{\Omega} f(\underline{x})\,dx \quad \Omega \subseteq \mathbb{R}^d$

① can use extensions of standard methods

② Markov integration

↳ idea: randomly sample

$$\int_{\Omega} f(x_1, \dots, x_d)\, d\Omega = \mathrm{Vol}(\Omega) \cdot \mathbb{E}_{\Omega}\big(f(\underbrace{x_1 \dots x_d}_{\substack{\text{random} \\ \text{vector} \\ \text{in } \mathbb{R}^d}})\big)$$

If we put a box where not all point lie in Ω (rejection sampling)

$$\int_{\Omega} f(x_1 \dots x_d)\, d\Omega = \frac{\mathrm{Vol}(\Omega)}{\mathrm{Vol}(\mathrm{box})} \mathbb{E}_{\Omega}\big(f(x_1 \dots x_d)\big)$$

Differential Equations

$$y' = f(x, y)$$
$$f(x_0) = y_0$$

Separable variables

$$\dot{x} = f(t)g(x) \Rightarrow \frac{dx}{dt} = f(t)g(x)$$
$$\int \frac{dx}{g(x)} = \int f(t)\,dt$$

Linear

$$y' + f(x)y = g(x) \qquad g(x) = 0 \Rightarrow \text{homogeneous}$$
$$\neq 0 \rightarrow \text{non-homogeneous}$$

① solve homogeneous

$$y' + f(x)y = 0 \Rightarrow y = Ce^{-\int f(x)dx}$$
$$= Cz(x)$$

② put homogeneous solution into original problem

$$y = C(x)z(x) \quad \text{Solve for } C(x)$$

Most we cannot solve symbolically

Numerical

$[a,b]$ $\quad y' = f(x,y) \quad y(a) = y_0$

Divide $[a,b]$

$$a = x_0 < x_1 < x_2 < \cdots < x_n = b$$

$h_i = x_{i+1} - x_i$

$y_i =$ approximation at x_i

$g_i = y_i - y(x_i)$ $\qquad z' = f(x,y)$

$\qquad\qquad\qquad\qquad z(x_{i-1}) = y_{i-1}$

$l_i = y_i - z(x_i)$ local error (one step)

global error

$$g_i \leq |l_1| + |l_2| + \cdots |l_i|$$

Order of the method: (definition)

$$l_i = C h_i^{p+1} + O(h_i^{p+2})$$

$\boxed{\text{order } p}$

Euler's method

- use linear approximation of function

- solution on interval $[x_i, x_{i+1}]$
  is replaced by tangent of solution
  at x_i

$$y_{i+1} = y_i + \underbrace{h_i}_{x_{i+1} - x_i} f(x_i, y_i)$$

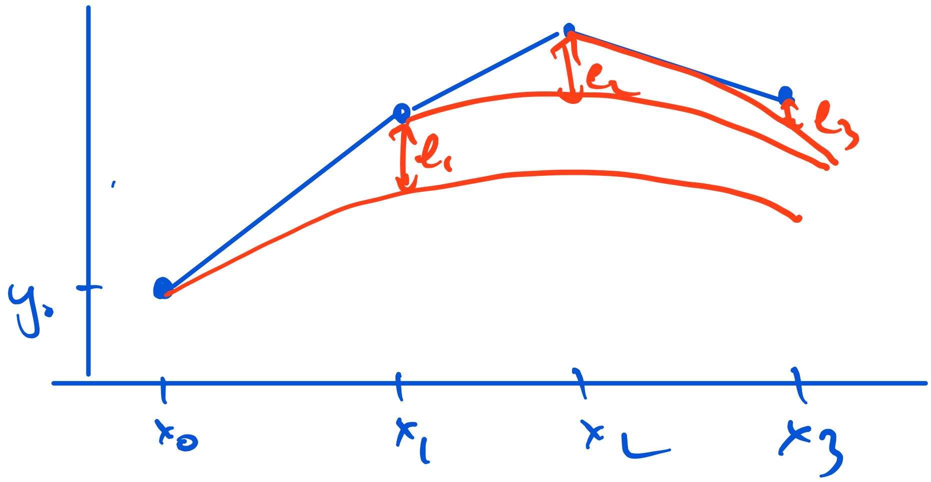
Alg

$y = y_0$
$x = x_0$
$h = \frac{b-a}{n}$

for $i = 1 \dots n-1$
$\quad y = y + h f(x,y)$
$\quad x = x + h$

where $y(x+h) = \underbrace{y(x) + h y'(x)}_{\text{used for update}} + \underbrace{\frac{h}{2} y''(\xi)}_{\text{error}}$

Example



order of Euler's method is 1

local error is $O(h^2)$

global error is $O(h)$

Runga-Kutta (order 2)

Idea - take weighted average of slopes rather than a single estimate

Example

x_n & $x_n + ch$ $[x_n, x_{n+1}]$

$h = x_{n+1} - x_n$; $c \in [0, 1]$

$y_{n+1} \leftarrow$ move by expected average tangents at x_n & $x_n + ch$

$$y_{n+1} = y_n + \underset{\substack{\uparrow \\ \text{weight}}}{b_1} \overbrace{(hf(x_n, y_n))}^{\text{tangent at } x_n} +$$

$$b_2 \underbrace{(hf(x_n + ch, y(x_n + ch)))}_{\text{tangent at } x_n + ch}$$

where $y(x_n + ch) \approx y_n + ch y'(x_n)$

$= y_n + chf(x_n, y_n)$

$\approx y_n + \underset{\substack{\uparrow \\ \text{free parameter}}}{a} hf(x_n, y_n)$

Substitute in

$$y_{n+1} = y_n + b_1 \underbrace{h f(x_n, y_n)}_{k_1} + b_2 \underbrace{h f(x_n + ch, y_n + a k_1)}_{k_2}$$

expand $y(x_n + ch)$ & $f(x_n + ch, y_n + a k_1)$

w/ Taylor expansion & compare

coefficients for h & h^2

$$\Rightarrow \quad 1 = b_1 + b_2$$

$$\tfrac{1}{2}(f_x + f_y \cdot f)_n = b_1 c (f_x)_n + b_2 a (f_y)_n$$

where $f_n = f(x_n, y_n)$

$$(f_x)_n = \underset{\substack{\uparrow \\ \text{derivative} \\ \text{wrt } x}}{f_x}(x_n, y_n)$$

$$(f_y)_n = f_y(x_n, y_n)$$

Many solutions

Ex 1

$b_1 = b_2 = 1/2 \qquad c = a = 1$

$y_{n+1} = y_n + 1/2(k_1 + k_2)$

$k_1 = h f(x_n, y_n)$

$k_2 = h f(x_n + h, y_n + k_1)$

Ex 2

$b_1 = 1,\ b_2 = 0 \qquad c = a = 1/2$

$y_{n+1} = y_n + k_2$

$k_1 = h f(x_n, y_n)$

$k_2 = h f(x_n + 1/2\, h, y_n + 1/2\, k_1)$

General

$y_{n+1} = y_n + b_1 k_1 + b_2 k_2 + \dots + b_s k_s$

$k_1 = h f(x_n, y_n)$

$k_2 = h f(x_n + c_2 h, y_n + a_{2,1} k_1)$

$k_3 = h f(x_n + c_3 h, y_n + a_{3,1} k_1 + a_{3,2} k_2)$

$\vdots$

$k_s = h f(x_n + c_s h, y_n + a_{s,1} k_1 + \dots + a_{s,s-1} k_{s-1})$

Compact form: Butcher Tableau

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
c_2 & a_{2,1} & 0 & & & & \\
c_3 & a_{3,1} & a_{3,2} & 0 & & & \\
\vdots & \vdots & & & & & \\
c_s & a_{s,1} & a_{s,2} & \cdots & & a_{s,s-1} & 0 \\
\hline
 & b_1 & b_2 & & & b_{s-1} & b_s
\end{array}
$$

where $c_2 = a_{2,1}$

$$c_3 = a_{3,1} + a_{3,2}$$

$$\vdots$$

$$c_s = a_{s,1} + \cdots + a_{s,s-1}$$

Most popular — order 4

$$
\begin{array}{c|cccc}
0 & 0 & & & \\
\frac{1}{2} & \frac{1}{2} & 0 & & \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 & \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
$$

$$y_{n+1} = y_n + \frac{1}{6}k_1 + \frac{1}{3}k_2 + \frac{1}{3}k_3 + \frac{1}{6}k_4$$

$$k_1 = hf(x_n, y_n)$$

$$k_2 = hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_1)$$

$$k_3 = hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_2)$$

$$k_4 = hf(x_n + h, y_n + k_3)$$

Error estimates

- we care about global error
- estimate local error
  - ↳ use this to determine step size

Method M of order p

$$l_{n+1} = y_{n+1,h} - z(x_{n+1}) \approx Ch^{p+1}$$

$z(x) \Rightarrow$ solution

$$y' = f(x,y) \quad y(x_n) = y_n$$

But at $h/2$

2 steps to get to h

$$l_{n+1} = y_{n+1,h/2} - z(x_{n+1}) \approx C(h/2)^{p+1} + C(h/2)^{p+1}$$

$$= 2^{-p} Ch^{p+1}$$

$$y_{n+1,h} - y_{n+1,h/2} \approx Ch^{p+1}(1-2^{-p})$$

$$Ch^{p+1} \approx \frac{y_{n+1,h} - y_{n+1,h/2}}{1-2^{-p}}$$

1. if $|l_{n+1}| < \varepsilon h$ → use $y_{n+1,h}$

   (if we used $y_{n+1,h/2}$ we need to use it twice)

   use h going forward

2. if $|l_{n+1}| > \varepsilon h$ => shorter step

3. if $|l_{n+1}| \ll \varepsilon h$ => lengthen step

<u>How</u>

$$l_n \approx C h_n^{p+1}$$

$$C h_{n+1}^{p+1} \approx \varepsilon h_{n+1}$$

$$\frac{h_{n+1}^{p+1}}{h_n^{p+1}} \approx \frac{\varepsilon h_{n+1}}{|l_n|}$$

* multiply by $\sigma \approx 1$ to mitigate numerical error (e.g. $\sigma = 0.9$)

example

next step should be

$$h_{n+1}^{p+1} = h_n \left(\frac{\varepsilon h_n}{|l_n|} \right)^{1/p}$$