

# Adaptive Simpson

## CS/SE 4X03

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# Outline

# Derivation of Simpson's rule

Simpson's rule can be derived using the method of undetermined coefficients

- Seek integration formula of the form

$$\int_a^b f(x)dx \approx Af(a) + Bf\left(\frac{a+b}{2}\right) + Cf(b)$$

- Find  $A$ ,  $B$ ,  $C$  such that for quadratic polynomials the formula is exact:

$$\int_a^b f(x)dx = Af(a) + Bf\left(\frac{a+b}{2}\right) + Cf(b)$$

## Derivation of Simpson's rule cont.

- Let  $a = -1$ ,  $b = 1$ . We should integrate exactly  $1$ ,  $x$ ,  $x^2$ :

$$f(x) = 1 : \int_{-1}^1 dx = 2 = A + B + C$$

$$f(x) = x : \int_{-1}^1 x dx = 0 = -A + C$$

$$f(x) = x^2 : \int_{-1}^1 x^2 dx = \frac{2}{3} = A + C$$

from which  $A = 1/3$ ,  $C = 1/3$ ,  $B = 4/3$

- Hence

$$\int_{-1}^1 f(x) dx \approx \frac{1}{3} [f(-1) + 4f(0) + f(1)]$$

## Derivation of Simpson's rule cont.

- Let  $y(x) = 0.5(b - a)x + 0.5(b + a)$ ,  $y(-1) = a$ ,  $y(1) = b$
- Changing variables:

$$\int_a^b f(x)dx \approx \frac{b-a}{6} \left[ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

# Adaptive Simpson

- Given a function  $f(x)$  on  $[a, b]$  and tolerance  $\text{tol}$
- find  $Q$  such that

$$|Q - I| \leq \text{tol},$$

where

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

## Adaptive Simpson cont.

Denote  $h = b - a$ . Then

$$I = \int_a^b f(x)dx = S(a, b) + E(a, b),$$

where

$$S(a, b) = \frac{h}{6} \left[ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$
$$E(a, b) = -\frac{1}{90} \left(\frac{h}{2}\right)^5 f^{(4)}(\xi), \quad \xi \text{ between } a \text{ and } b$$

Denote  $S_1 = S(a, b)$  and  $E_1 = E(a, b)$

## Adaptive Simpson cont.

- Let  $c = (a + b)/2$  and apply Simpson on  $[a, c]$  and  $[c, b]$ :

$$I = \int_a^b f(x)dx = \underbrace{S(a, c) + S(c, b)}_{S_2} + \underbrace{E(a, c) + E(c, b)}_{E_2}$$

- We can compute  $S_1$  and  $S_2$
- How to estimate the error? If  $f^{(4)}$  does not change much on  $[a, b]$

$$\begin{aligned} E(a, c) &= -\frac{1}{90} \left( \frac{h/2}{2} \right)^5 f^{(4)}(\xi_1) = \frac{1}{32} \left[ -\frac{1}{90} \left( \frac{h}{2} \right)^5 f^{(4)}(\xi_1) \right], \quad \xi_1 \in [a, c] \\ &\approx \frac{1}{32} \left[ -\frac{1}{90} \left( \frac{h}{2} \right)^5 f^{(4)}(\xi) \right] \\ &= \frac{1}{32} E_1 \end{aligned}$$



## Adaptive Simpson cont.

Similarly  $E(c, b) \approx \frac{1}{32}E_1$

- Hence

$$E_2 = E(a, c) + E(c, b) \approx \frac{1}{16}E_1$$

- From  $I = S_1 + E_1 = S_2 + E_2$ ,

$$S_1 - S_2 = E_2 - E_1 \approx E_2 - 16E_2 = -15E_2$$

$$E_2 \approx \frac{1}{15}(S_2 - S_1)$$

- Then

$$I = \int_a^b f(x)dx = S_2 + E_2 \approx S_2 + \frac{1}{15}(S_2 - S_1)$$

# Method outline

Given  $f$ ,  $[a, b]$  and  $\text{tol}$ :

- $c = (a + b)/2$
- Compute  $S_1 = S(a, b)$  and  $S_2 = S(a, c) + S(c, b)$
- $E_2 = (S_2 - S_1)/15$
- If  $|E_2| \leq \text{tol}$  return  $S_2 + E_2$   
else apply recursively on  $[a, c]$  and  $[c, b]$

## Adaptive Simpson cont.

*Algorithm 2.1 (Adaptive Simpson).*

$S = \text{quadSimpson}(f, a, b, \text{tol})$

$$h = b - a, c = (a + b)/2$$

$$S_1 = \frac{h}{6} [f(a) + 4f(\frac{a+b}{2}) + f(b)]$$

$$S_2 = \frac{h}{12} [f(a) + 4f(\frac{a+c}{2}) + 2f(c) + 4f(\frac{c+b}{2}) + f(b)]$$

$$E_2 = \frac{1}{15}(S_2 - S_1)$$

if  $|E_2| \leq \text{tol}$

    return  $S_2 + E_2$

else

$$Q_1 = \text{quadSimpson}(f, a, c, \text{tol}/2)$$

$$Q_2 = \text{quadSimpson}(f, c, b, \text{tol}/2)$$

$$\text{return } Q_1 + Q_2$$

## Why it works

- Let  $I = \int_a^b f(x)dx$ ,  $I_1 = \int_a^c f(x)dx$ ,  $I_2 = \int_b^c f(x)dx$
- If  $|I_1 - Q_1| \leq \text{tol} / 2$  and  $|I_2 - Q_2| \leq \text{tol} / 2$ , then

$$\begin{aligned}|I - Q| &= |(I_1 + I_2) - (Q_1 + Q_2)| \\&= |I_1 - Q_1 + I_2 - Q_2| \\&\leq |I_1 - Q_1| + |I_2 - Q_2| \\&\leq \text{tol} / 2 + \text{tol} / 2 \\&= \text{tol}\end{aligned}$$

# Subtleties

- The error estimate assumes  $f^{(4)}$  does not vary much, but it may, and then this estimate may not be accurate  
To compensate in such cases, include a safety factor, e.g.

$$|E_1| \leq 10 \times \text{tol}$$

- The recursion may run “deep” if  $\text{tol}$  is too small or  $f^{(4)}$  varies a lot  
Insert a counter to stop the recursion when the depth exceeds some number, e.g. 20