Adaptive Simpson

CS/SE 4X03

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October 25, 2021

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:

$$
\begin{aligned}
f(x) = 1: &\quad \int_{-1}^{1} dx = 2 = A + B + C \\
f(x) = x: &\quad \int_{-1}^{1} x dx = 0 = -A + C \\
f(x) = x^2: &\quad \int_{-1}^{1} x^2 dx = \frac{2}{3} = A + C
\end{aligned}
$$

  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 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.

a c b

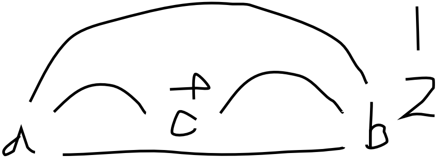
- Let $c = (a+b)/2$ and apply Simpson on $[a, c]$ and $[c, b]$:

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

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

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

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

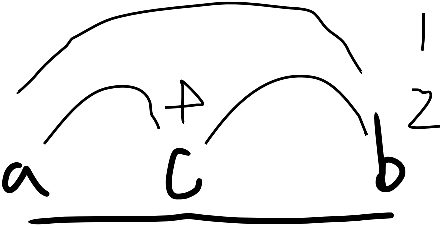
$$I = \int_a^b f(x)dx = S_2 + E_2 \approx S_2 + \frac{1}{15}(S_2 - S_1)$$

Method outline

Given f, $[a,b]$ and 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 $|E_2| \le \text{tol}$ return $S_2 + E_2$
  else apply recursively on $[a,c]$ and $[c,b]$

Adaptive Simpson cont.



Algorithm 2.1 (Adaptive Simpson).

S = quadSimpson(f, a, b, 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 $|E_2| \leq$ tol

  return $S_2 + E_2$

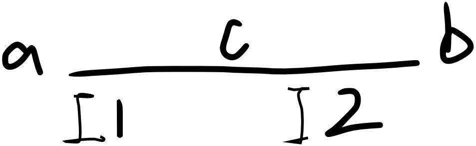
else

  Q_1 = quadSimpson(f, a, c, tol/2)

  Q_2 = quadSimpson(f, c, b, tol/2)

  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 $|I_1 - Q_1| \le$ tol $/2$ and $|I_2 - Q_2| \le$ tol $/2$, then ?

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

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 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