Last class:

* Newton-Cotes quadrature rules $(n=1, n=2)$ — replace integrand $f(x)$ with $P_n(x)$ and integrate $P_n(x)$

Today:

* error estimates
* composite formulae.

Trapezoid rule $(n=1)$

$$\int_a^b f(x)\,dx \simeq \int_a^b P_2(x)\,dx = \frac{b-a}{2}\left[f(a)+f(b)\right]$$

Simpson's rule $(n=2)$

$$\int_a^b f(x)\,dx \simeq \int_a^b P_2(x)\,dx = \frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]$$

Warning: Runge phenomenon can occur for large n.

$$\int_{-5}^{5} \frac{1}{1+x^2}\,dx \simeq \int_{-5}^{5} P_n(x)\,dx$$

error increases without bound for large n.

CURE: composite quadrature rules

ERROR ESTIMATES

We seek to study the error

$$E_n(f) = \int_a^b f(x)\,dx - \sum_{k=0}^{n} w_k f(x_k)$$

i.e., what is the size of the error that is being commited by integrating the lagrange interpolant?

$$|E_n(f)| = \left| \int_a^b f \, dx - \sum_{k=0}^{n} \omega_k f(x_k) \right|$$

$$= \left| \int_a^b f \, dx - \int_a^b P_n(x) \, dx \right|$$

$$= \left| \int_a^b f - P_n \, dx \right|$$

$$\leq \int_a^b \underbrace{|f(x) - P_n(x)|}_{} \, dx$$

RECALL:

$$|f(x) - P_n(x)| \leq \frac{M_{n+1}}{(n+1)!} |\pi_{n+1}(x)|$$

$$M_{n+1} = \max_{\xi \in [a,b]} |f^{(n+1)}(\xi)|$$

$$\leq \int_a^b \frac{M_{n+1}}{(n+1)!} |\pi_{n+1}(x)| \, dx$$

Now, we can use this estimate to determine an upper bound on the error commited when using the trapezoid rule $(n=1)$

$$|E_1(f)| \leq \frac{M_2}{2}\int_a^b |\pi_2(x)|\,dx$$

$$= \frac{M_2}{2}\int_a^b |\underbrace{(x-a)}_{+}\underbrace{(x-b)}_{-}|\,dx$$

$$= \frac{M_2}{2}\int_a^b (x-a)(b-x)\,dx$$

$$= \frac{(b-a)^3}{12} M_2$$

For Simpson's rule $(n=2)$

$$|E_2(f)| \leq \frac{M_3}{6}\int_a^b \left|(x-a)\left(x-\frac{(a+b)}{2}\right)(x-b)\right|dx$$

$$= \frac{(b-a)^4}{196} M_3$$

A considerable over estimate

NOTE: $E_1(f)=0$ when $f \in P_1$

$E_2(f)=0$ when $f \in P_2$, $\boxed{f \in P_3}$ This is true too & can be shown

n odd, Newton-Cotes is exact for polynomials of order n

n is even, Newton-Cotes is exact for polynomials of order $n+1$.

Error bound is a considerable OVER estimate of the actual error. It does not reflect the fact that $E_2(f) = 0$ when $f \in P_3$.

Theorem: (improved) estimate for Simpson's rule:

$f : [a,b] \to \mathbb{R}$

$f^{(4)}$ exists and is continuous

then:

$$\int_a^b f(x)\,dx - \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] = -\frac{(b-a)^5}{2880} f^{(4)}(\xi) \quad ; \quad \xi \in (a,b)$$

$$|E_2(f)| \leq \frac{(b-a)^5}{2880} M_4 \qquad M_4 = \max_{x \in [a,b]} |f^{(4)}(x)|$$

This error bound correctly shows that $E_2(f) = 0$ when f is a polynomial of degree 3.

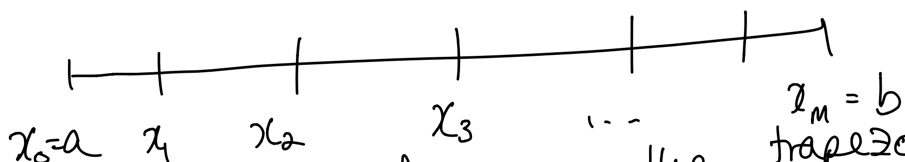
Composite formulae.

Subdivide the interval $[a,b]$ into smaller, equal sized subintervals, and use Newton-Cotes on each subinterval.

For example, select an $m \geq 2$, and divide $[a,b]$ into m subintervals.

$$\int_a^b f(x)\,dx = \sum_{i=1}^{m} \int_{x_{i-1}}^{x_i} f(x)\,dx$$

where $\quad x_i = a + \frac{i}{m}(b-a) \quad i = 0, 1, \ldots, m. \; ; \quad h = \frac{(b-a)}{m}$



On each subinterval, use the trapezoid rule.

$$\int_{x_{i-1}}^{x_i} f(x)\,dx \simeq \frac{1}{2} h \left[f(x_{i-1}) + f(x_i) \right]$$

$$\sum_{i=1}^{m} \int_{x_{i-1}}^{x_i} f(x)\,dx \approx \sum_{i=1}^{m} \frac{1}{2} h \left[f(x_{i-1}) + f(x_i) \right]$$

COMPOSITE TRAPEZOID RULE:

$$= h\left[\frac{1}{2} f(x_0) + f(x_1) + \dots + f(x_{m-1}) + \frac{1}{2} f(x_m) \right].$$

Error estimate:

$$\mathcal{E}_1(f) = \int_a^b f(x)\,dx - h\left[\frac{1}{2} f(x_0) + f(x_1) + \dots + f(x_{m-1}) + \frac{1}{2} f(x_m) \right]$$

$$= \sum_{i=1}^{m} \left\{ \int_{x_{i-1}}^{x_i} f(x)\,dx - \frac{1}{2} h \left[f(x_{i-1}) + f(x_i) \right] \right\}$$

Recall: $|E_1(f)| \le \frac{h^3}{12} \max_{\xi \in [x_{i-1}, x_i]} |f^{(2)}(\xi)|$

Take absolute value of both sides

$$|\mathcal{E}_1(f)| \le \sum_{i=1}^{m} \frac{1}{12} h^3 \max_{\xi \in [x_{i-1}, x_i]} |f^{(2)}(\xi)|$$

$$= \frac{1}{12} h^3 \sum_{i=1}^{m} \max_{\xi \in [x_{i-1}, x_i]} |f^{(2)}(\xi)|$$

$$= \frac{1}{12} h^3 \, m \, M_2 \quad ; \quad M_2 = \max_{\xi \in [a,b]} |f^{(2)}(\xi)|$$

$$= \frac{1}{12} \left(\frac{b-a}{m} \right)^3 m \, M_2$$

$$= \frac{1}{12} \frac{(b-a)^3}{m^2} M_2$$

Composite Simpson's Rule

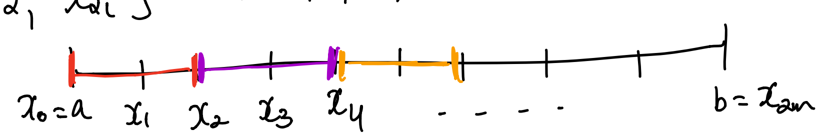
Let us suppose that $[a,b]$ now is divided into $2m$ intervals with the points

$$x_i = a + i \, \frac{b-a}{2m} \; ; \quad i = 0, 1, 2, \ldots, 2m$$

$$h = \frac{b-a}{2m}$$

and Simpson's rule is applied to each interval

$[x_{2i-2}, x_{2i}]$ $\quad i = 1, 2, \ldots, m$.



Simpson's rule on each subinterval.

$$\int_a^b f(x)\,dx = \sum_{i=1}^{m} \int_{x_{2i-2}}^{x_{2i}} f(x)\,dx$$

$$\approx \sum_{i=1}^{m} \frac{2h}{6}\left[f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})\right]$$

$$= \frac{h}{3}\Big[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \dots + 2f(x_{2m-2}) + 4f(x_{2m-1}) + f(x_{2m})\Big].$$

Error Estimate:

$$|\mathcal{E}_2(f)| \le \underbrace{\frac{(b-a)^5}{2880\,m^4} M_4}_{\text{zero for } f \in \mathcal{P}_3} \; ; \quad M_4 = \max_{\xi \in [a,b]} |f^{(4)}(\xi)|$$

Remark: Composite formulae are more accurate than the Newton–Cotes formulae

AS LONG AS f is SUFFICIENTLY SMOOTH, THE ERROR CAN BE MADE ARBITRARILY SMALL BY CHOOSING ENOUGH SUBINTERVALS.