Last class: * Lagrange interpolation

* Hermite interpolation (finish)

* Numerical integration (start)

$x_0, x_1, \dots, x_n \in \mathbb{R}$ (distinct)

$y_0, y_1, \dots, y_n \in \mathbb{R}$

$z_0, z_1, \dots, z_n \in \mathbb{R}$

Find $p_{2n+1} \in \mathcal{P}_{2n+1}$ such that $p_{2n+1}(x_i) = y_i$, $p'_{2n+1}(x_i) = z_i$ $\quad i = 0, \dots, n$

$$\boxed{p_{2n+1}(x) = \sum_{k=0}^{n} H_k(x) y_k + K_k(x) z_k}$$

is the Hermite interpolation polynomial

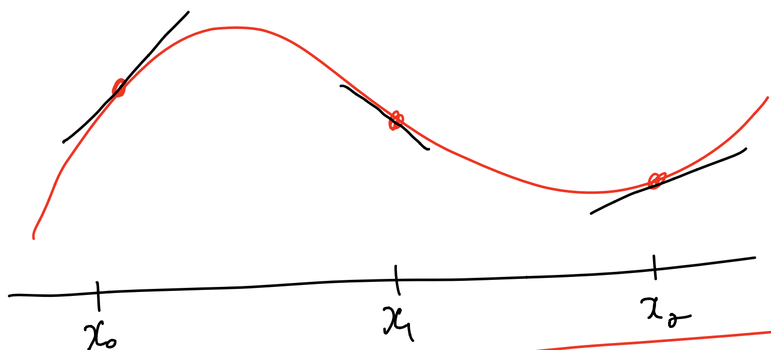
What properties of H_k and K_k do we expect?

$$\begin{cases} H_k(x_i) = \begin{cases} 1 & i = k \\ 0 & i \neq k \end{cases} \\ H'_k(x_i) = 0 \end{cases} \qquad \begin{cases} K_k(x_i) = 0 \\ K'_k(x_i) = \begin{cases} 1 & i = k \\ 0 & i \neq k \end{cases} \end{cases}$$

$$H_k(x) = (L_k(x))^2\left(1 - 2L_k'(x_k)(x-x_k)\right) \in \mathcal{P}_{2n+1}$$

$$K_k(x) = (L_k(x))^2(x-x_k) \in \mathcal{P}_{2n+1}$$

satisfy the above constraints



Theorem: $n \geq 0$, $f:[a,b]\to\mathbb{R}$, $f^{(2n+2)}$ is continuous, then the (unique) Hermite interpolant of f satisfies

$$f(x) - P_{2n+1}(x) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!}\left(\pi_{n+1}(x)\right)^2;$$

$$\pi_{n+1}(x) = \prod_{k=0}^{n}(x-x_k)$$

$$\left|f(x) - P_{2n+1}(x)\right| \leq \frac{M_{2n+2}}{(2n+2)!}\left(\pi_{n+1}(x)\right)^2$$

PROOF: see Süli

Example: For $n=1$, construct a cubic polynomial P_3 such that

$$P_3(0) = \overset{y_0}{0} \qquad P_3(1) = \overset{z_0}{1} \qquad P_3'(0) = \overset{y_1}{1} \qquad P_3'(1) = \overset{z_1}{0}$$

$x_0 = 0 \qquad x_1 = 1$

$$P_3(x) = H_0(x)\underset{\overset{\|}{0}}{y_0} + K_0(x)\underset{\overset{\|}{1}}{z_0} + H_1(x)\underset{\overset{\|}{1}}{y_1} + K_1(x)\underset{\overset{\|}{0}}{z_1}$$

$$= K_0(x) + H_1(x)$$

$L_0(x) = 1 - x \qquad L_1(x) = x$ for $x_0 = 0 \quad x_1 = 1$

$K_0(x) = [L_0(x)]^2 (x - x_0) = (1-x)^2 x$

$H_1(x) = [L_1(x)]^2 (1 - 2L_1'(x_1)(x - x_1)) = x^2(3 - 2x)$

$\Rightarrow \quad P_3(x) = -x^3 + x^2 + x$

Using the interpolant (e.g. Lagrange) to compute approximate derivatives to f.

How accurately does $P_n'(x)$ approximate $f'(x)$?

Numerical differentiation

Recall

$$f(x) - P_n(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \pi_{n+1}(x)$$

We can try to differentiate the above, except... it's not clear that $\xi(x)$ is continuous, or even differentiable.

If p_n is Lagrange interpolant of f on $[a,b]$, we have

$$|f'(x) - p_n'(x)| \leq \frac{(b-a)^n}{n!} M_{n+1}$$

(for proof see Süli)

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

If $\lim_{n \to \infty} \frac{(b-a)^n}{n!} M_{n+1} = 0$, then $p_n' \to f'$ uniformly on $[a,b]$

Numerical Integration

The definite integrals

$$\int_0^1 e^x \, dx \quad \text{and} \quad \int_0^\pi \cos(x) \, dx$$

are easy to evaluate analytically.

Unfortunately, most integrals cannot be evaluated analytically (with for example a table of integrals).

For example:

$$\int_0^1 e^{x^2}\,dx \quad \text{and} \quad \int_0^{\pi} \cos(x^2)\,dx$$

Now, for general integrals

$$\int_a^b f(x)\,dx,$$

since polynomials are easy to integrate, the idea is to replace f with a polynomial and integrate the polynomial exactly.

Newton - Cotes Formulae

Replace $f(x)$ with its Lagrange interpolant of degree n.

all that is required is the function values $f(x_i)$

$$\int_a^b f(x)\,dx \approx \int_a^b P_n(x)\,dx \; ; \quad \text{where the}$$

interpolation points, $x_i = a + \frac{(b-a)}{n} i \quad i = 0, 1, 2, \ldots, n,$

are equidistant.

Recall $P_n(x) = \sum_{k=0}^{n} L_k(x) f(x_k)$; $L_k(x) = \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{(x - x_i)}{(x_k - x_i)}$

$$\int_a^b f(x)\,dx \approx \int_a^b \sum_{k=0}^{n} L_k(x) f(x_k)\,dx$$

$$= \sum_{k=0}^{n} f(x_k) \underbrace{\int_a^b L_k(x)\,dx}_{\substack{\text{can be easily} \\ \text{precomputed, exactly.} \\ \text{"weights", } w_k}}$$

$$= \sum_{k=0}^{n} w_k f(x_k)$$

With above choices, we obtain a Newton-Cotes formula of order n.

w_k : quadrature weights
x_k : quadrature points

$\Big\}$ quadrature rule

For $n=1$: Trapezoid rule

$$\int_a^b f(x)\,dx \approx \int_a^b P_1(x)\,dx$$

$$x_i = a + \frac{(b-a)}{n} i \Rightarrow x_0 = a, \quad x_1 = b$$

$$P_1(x) = L_0(x) f(a) + L_1(x) f(b)$$

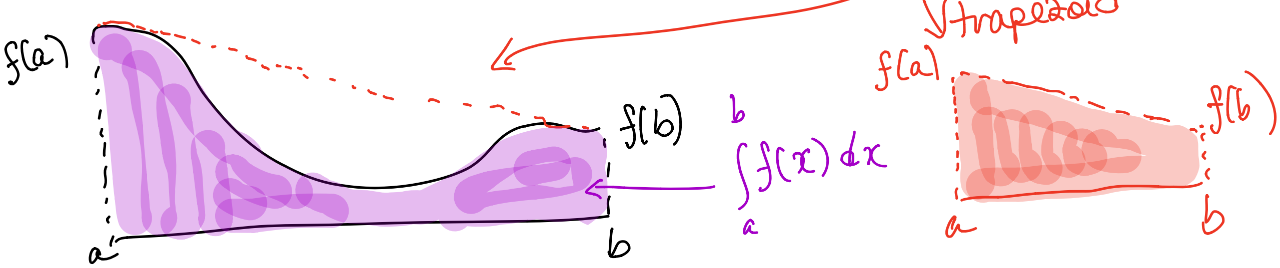
$$= \frac{x-b}{a-b} f(a) + \frac{x-a}{b-a} f(b)$$

$$= \frac{1}{b-a}\left\{ (b-x) f(a) + (x-a) f(b) \right\}$$

$$\int_a^b P_1(x)\,dx = \frac{1}{b-a}\left\{ f(a)\int_a^b b-x\,dx + f(b)\int_a^b x-a\,dx \right\}$$

$$= \frac{b-a}{2}\left[f(a) + f(b) \right]$$

area of the trapezoid



$x_0 = a$ $\qquad x_1 = b$ $\qquad (w_0, x_0)$

$w_0 = \frac{b-a}{2}$ $\qquad w_1 = \frac{b-a}{2}$ $\qquad (w_0, x_1)$

For $n=2$: Simpson's Rule

$$x_i = a + \frac{(b-a)}{n} i \Rightarrow x_0 = a, \; x_1 = \frac{b-a}{2}, \; x_2 = b$$

$$\int_a^b f(x)\,dx = \int_a^b f(x_0)L_0 + f(x_1)L_1 + f(x_2)L_2 \, dx$$

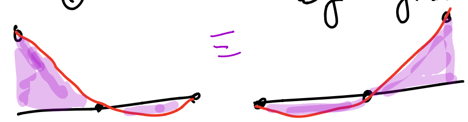
$$w_0 = \int_a^b L_0(x)\,dx = \int_a^b \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}\,dx$$

evaluate the integral with the change of variables

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

$$= \int_{-1}^{1} \frac{t(t-1)}{2} \frac{b-a}{2}\,dt = \frac{b-a}{6} = w_0 = w_2$$

by symmetry



Remark: you could use the change of variables, or, more simply, expand the product

$$\underbrace{\frac{1}{(x_0-x_1)(x_0-x_2)}}_{\text{constant}} \left\{ x^2 - (x_1+x_2)x + x_1 x_2 \right\}$$

and integrate each term separately

You can also compute $w_1 = \frac{4}{6}(b-a)$

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

Since the weights are independent of f, they can be precomputed in advanced.

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 $(n=1)$

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

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

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

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

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

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

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

NOTE: $E_1(f)=0$ when $f \in \mathcal{P}_1$

$E_2(f)=0$ when $f \in \mathcal{P}_2$, $f \in \mathcal{P}_3$

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 $n+1$.

Next class: composite quadrature rules.