Numerical Quadrature

Summary From last time:

Lagrange Interpolant: $p_n(x) = \sum_{k=0}^{n} f(x_k) L_k(x)$

Hermite Interpolant:

$$p_{2n+1}(x) = \sum_{k=0}^{n} f(x_k) H_k(x) + f'(x_k) K_k(x).$$

Here: $$L_k(x) = \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{x - x_i}{x_k - x_i}$$

$$H_k(x) = \left(L_k(x)\right)^2 \left(1 - 2L_k'(x_k)(x - x_k)\right)$$

$$K_k(x) = \left(L_k(x)\right)^2 (x - x_k).$$

By construction: $p_n(x_i) = f(x_i)$ Lagrange

and

Hermite $\begin{cases} p_{2n+1}(x_i) = f(x_i) \\ p_{2n+1}'(x_i) = f'(x_i). \end{cases}$

→ Lagrange and Hermite interpolation theorems: p_n and p_{2n+1} are the unique polys in $\mathcal{P}_n$ and $\mathcal{P}_{2n+1}$ respectively which satisfy those interpolation conditions.

What about the "error"?

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

and

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

$$\pi_{n+1} = (x - x_0) \cdots (x - x_n)$$

How about approximating the derivative of f?

Differentiate p_n: $\displaystyle p_n'(x) = \sum_{k=0}^{n} f(x_k) L_k'(x).$

Thm 6.6 $\quad n \geq 1$

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

These integrals are simple:

$$\int_0^1 e^x \, dx \quad , \quad \int_0^\pi \cos x \, dx.$$

These are not:

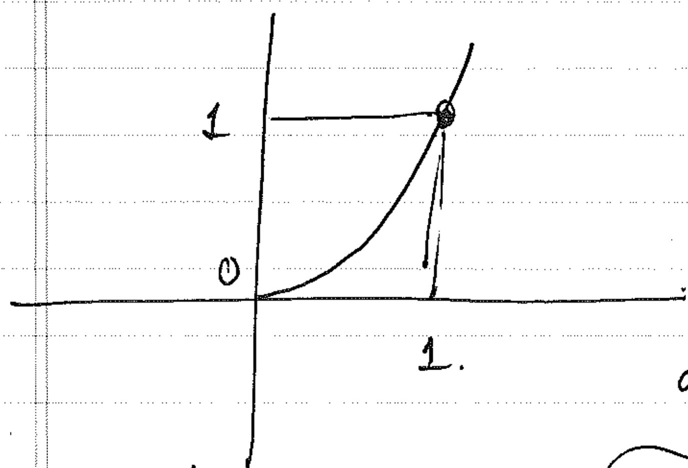
$$\int_0^1 e^{x^2} dx \quad , \quad \int_0^\pi \cos(x^2)\, dx$$

or this:

$$\int_1^{2000} \exp(\sin(\cos(\sinh(\cosh(\tan^{-1}(\log x)))))) \, dx$$

We want to approximate these latter integrals numerically.

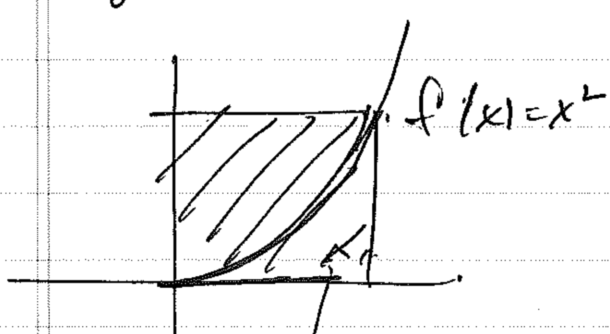
<u>Example:</u> $f(x) = x^2$.



$$\int_0^1 f(x) \approx \overbrace{\underbrace{(1-0)}_{\text{width of interval}} \cdot \underbrace{f(0)}_{\text{function value}}}^{\text{area of rectangle}} = 0.$$

<u>or</u>

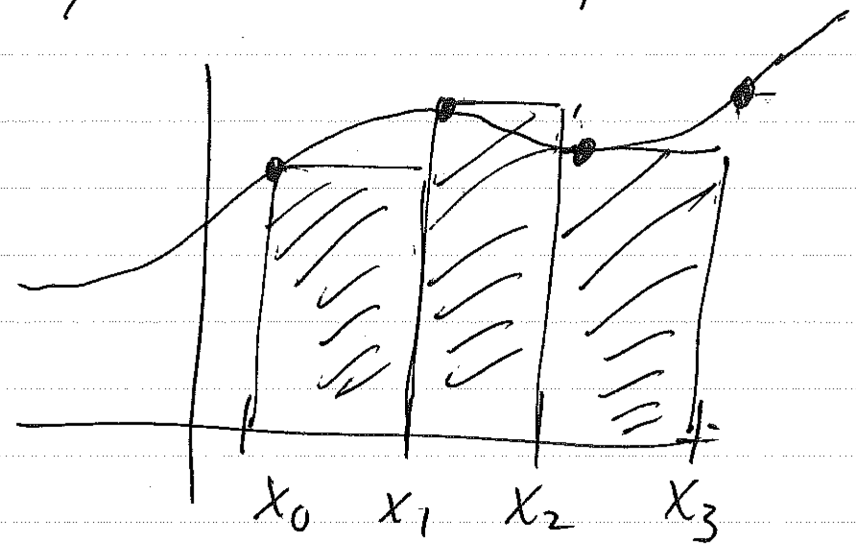
$$\int_0^1 f(x) \approx (1-0)\, f(1) = 1.$$



$= (1-0)\, f(1).$

A bit more generally:

Lay out a set of points: x_i, $i = 0, \ldots, n$



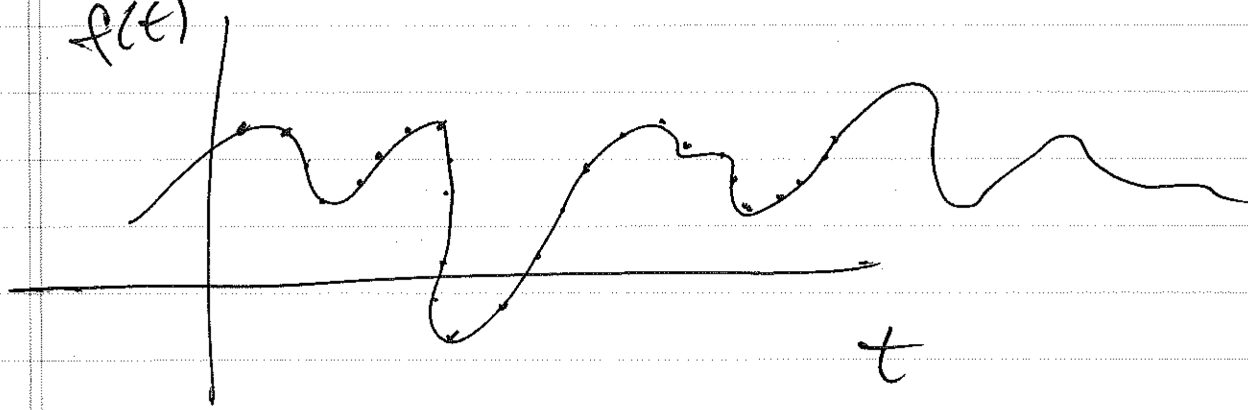
$$\int_{x_0}^{x_3} f(x)\,dx \approx A_1 + A_2 + A_3$$

$$A_i = \text{area of rectangle } i$$
$$= (x_{i+1} - x_i)\, f(x_i).$$

Note that you could use rectangles with different heights

$$A_i = (x_{i+1} - x_i) \underbrace{f(x_{i+1})}_{\text{instead of } f(x_i)}.$$

<u>Example:</u> Given a discrete time series, compute an average of some interval of length T.



Spacing between points in Δt.

Pick N so that $T = N\Delta t$.

$$\overline{f} = \frac{1}{N}\sum_{i=1}^{N} f(t_i).$$

$$= \frac{1}{N\Delta t} \sum_{i=1}^{N} \Delta t\, f(t_i)$$

$$= \frac{1}{T} \sum_{i=1}^{N} \Delta t\, f(t_i)$$

$$\approx \frac{1}{T} \int_0^T f(t)\, dt.$$

Newton-Cotes formulas:

→ Idea; use a Lagrange interpolation poly for integration:

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

Let's assume our interpolation pts are evenly spaced:

$$x_i = a + ih, \quad i = 0, \dots, n$$

$$h = \frac{b-a}{n}.$$

Recall: $p_n(x) = \sum_{k=0}^{n} f(x_k) L_k(x).$

So, we have $\int_a^b f(x)\,dx \approx \int_a^b p_n(x)\,dx$

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

$$= \sum_{k=0}^{n} f(x_k) \underbrace{\left(\int_a^b L_k(x)\,dx \right)}_{= w_k},$$

"~~interpolation~~ quadrature weights",

x_i = these are now called "quadrature points."

Trapezoid Rule: $n = 1$, so $x_0 = a, x_1 = b$.

$$p_1(x) = L_0(x) f(a) + L_1(x) f(b).$$

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

$$= \frac{1}{b-a}\Big((b-x) f(a) + (x-a) f(b) \Big).$$

$$\int_a^b p_1(x)\,dx = \frac{f(a)}{b-a}\int_a^b (b-x)\,dx + \frac{f(b)}{b-a}\int_a^b (x-a)\,dx$$

$$= \frac{f(a)}{b-a}\left(bx - \frac{1}{2}x^2 \Big|_a^b \right) + \frac{f(b)}{b-a}\left(\frac{1}{2}x^2 - ax \Big|_a^b \right)$$

$$= \frac{f(a)}{b-a}\left(b^2 - \frac{1}{2}b^2 - ab + \frac{1}{2}a^2 \right)$$

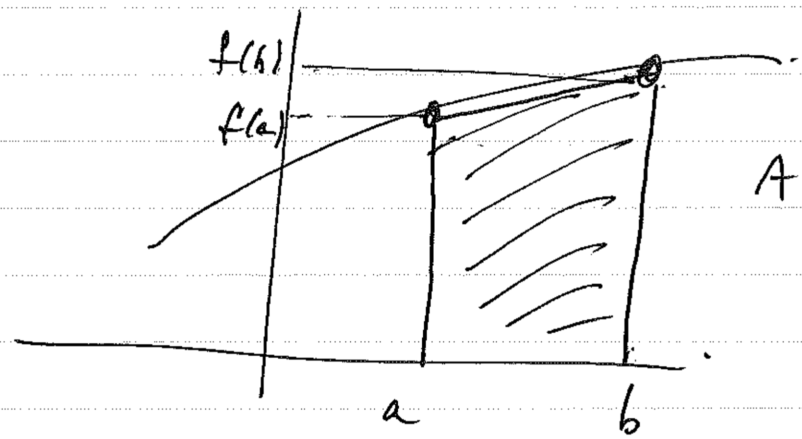
$$+ \frac{f(b)}{b-a}\left(\frac{1}{2}b^2 - ab - \frac{1}{2}a^2 + a^2 \right)$$

$$= \frac{f(a)}{b-a}\left(\frac{1}{2}\left(\cancel{b^2} - a \right)^2 \right)$$

$$+ \frac{f(b)}{b-a}\left(\frac{1}{2}\left(b - a \right)^2 \right)$$

$$= \frac{b-a}{2}\Big(f(a) + f(b) \Big).$$

Geometrically, we are just computing the area of a trapezoid:



$$A = \frac{f(a)+f(b)}{2} h.$$

$$= \frac{f(a)+f(b)}{2}(b-a).$$

<u>Simpson's rule:</u> $n=2$. so

$$x_0 = a, \quad x_1 = \frac{a+b}{2}, \quad x_2 = b.$$

Let's compute the quadrature weights explicitly:

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

Change of variables to t:

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

$$a \le x \le b \iff -1 \le t \le 1.$$

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

$$= \frac{b-a}{6}.$$

You can show: $w_1 = \frac{4}{6}(b-a)$.

By symmetry $w_0 = w_2$.

So, Simpson's rule:

$$\int_a^b f(x)\,dx \approx \int_a^b p_2(x)\,dx$$

$$= w_0 f(a) + w_1 f\left(\frac{a+b}{2}\right) + w_2 f(b)$$

$$= \frac{b-a}{6}\left(f(a) + 4 f\left(\frac{a+b}{2}\right) + f(b)\right).$$

Error estimation:

Definition: The error (quadrature) is defined to be $E_n(f) = \int_a^b f(x)\,dx - \sum_{k=0}^{n} w_k f(x_k)$.

Thm: 7.1. $n \geq 1$.

$f^{(n+1)}$ cnts on $[a,b]$.

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

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

$$\pi_{n+1}(x) = (x-x_0) \cdots (x-x_n).$$

Pf: $$E_n(f) = \int_a^b f(x)\,dx - \int_a^b \left(\sum_{k=0}^{n} f(x_k) L_k(x)\right) dx$$

$$= \int_a^b \left(f(x) - p_n(x)\right) dx$$

$$= \int_a^b \frac{f^{(n+1)}(\xi)}{(n+1)!} \pi_{n+1}(x)\,dx$$

$$\Rightarrow |E_n(f)| = \left| \int_a^b \frac{f^{(n+1)}(\xi)}{(n+1)!} \pi_{n+1}(x)\,dx \right|$$

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

→ Application to Trapezoid Rule:

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

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

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

Note that if f is linear, then $M_2 = 0$, and $|E_1(f)| = 0$. i.e.

The Trapezoid rule is exact for linear function (degree 1 polys).

→ Application to Simpson's Rule:

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

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

Actually, Simpson's rule is <u>exact</u> for poly's of degree 3, so this is not a good estimate.

Rmk: If n is odd, Newton-Cotes formula is exact for polys of degree n.

(**) If n is even, Newton-Cotes is exact for polys of degree $n+1$!!!!

Sketch of proof for (**).

Step 1: Show that the quadrature weights for Newton-Cotes formula satisfy: $w_k = w_{n-k}$ for $k = 0, \ldots, n$.

Step 2: Consider the polynomial:

$g(x) = \left(x - \frac{a+b}{2}\right)^{n+1}$. Note that when n is even, $\frac{a+b}{2}$ is always the center quadrature node?. Also: For an arbitrary monic poly p_{n+1} of degree $n+1$:

$p_{n+1}(x) - g(x)$ is always a degree n poly since the x^{n+1} term cancels out.

So, we should be able to integrate $p_{n+1} - g$ exactly, with $n+1$ interpolation (quadrature nodes), i.e.

$$\sum_{k=0}^{n} w_k \left(p_{n+1}(x_k) - g(x_k)\right) = \int_a^b (p_{n+1} - g)\,dx$$

$$\Leftrightarrow \sum_{k=0}^{n} p_{n+1}(x_k) - \int_a^b p_{n+1}\,dx$$

$$= \underbrace{\sum_{k=0}^{n} w_k\, g(x_k)}_{=0} - \underbrace{\int_a^b g\,dx}_{=0}.$$