Lecture 22 — Numerical Analysis — April 19, 2018

Last time:

Numerical Integration

- trapezoidal rule
  - special case of Newton-Cotes Formulae

Idea: First interpolate f on $[a,b]$, then integrate the interpolant:

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

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

quadrature nodes

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

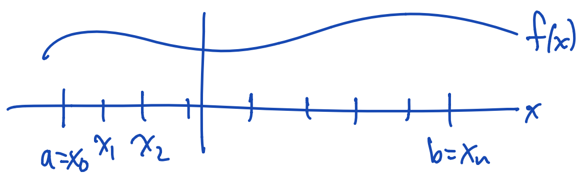
- for large n, w_k becomes expensive and the interpolant may suffer from Runge's Effect.

- Instead use lower-order, composite rules

The composite Trapezoidal Rule

Split the interval $[a,b]$ into n subintervals:

$$\int_a^b f = \int_{a=x_0}^{x_1} f + \int_{x_1}^{x_2} f + \dots + \int_{x_{n-1}}^{b=x_n} f$$



Apply the trapezoidal rule on each subinterval:

(assume equal size) $\quad x_{j+1} - x_j = \frac{b-a}{n} = h$.

Then $\displaystyle\int_a^b f(x)\,dx \approx T_n(f)$

$$= \sum_{j=1}^{n} h \cdot \left(\frac{f(x_{j-1}) + f(x_j)}{2} \right)$$

$$= h \left(\sum_{j=0}^{n} f(x_j) - \frac{1}{2}\left(f(a) + f(b)\right) \right)$$

The error can be shown to be $O(h^2)$.

In fact a formula exists that characterizes the error explicitly:

The Euler-Maclaurin Expansion

Thm: Let $f \in C^{2k}[a,b]$, and $[a,b]$ be divided into n subintervals, $[x_{i-1}, x_i]$, with

$$x_i = a + ih, \quad h = \frac{b-a}{n}.$$

Then

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

$$= \sum_{r=1}^{k} c_r h^{2r} \left(f^{(2r-1)}(b) - f^{(2r-1)}(a) \right) - d_{2k} \left(\frac{h}{2} \right)^{2k}$$

$$= \frac{h^2}{12}\left(f'(b) - f'(a)\right) - \frac{h^4}{720}\left(f^{(3)}(b) - f^{(3)}(a)\right) + \dots + (-1)^{k-1} \frac{B_{2n}}{(2k)!} h^{2k} f^{(2k)}(\xi)$$

$\ni \xi \in [a,b]$.

Fun fact: $c_r = -\frac{B_{2r}}{(2r)!}$, B_{2r} is a Bernoulli number:

$$\frac{x}{2}\coth\left(\frac{x}{2}\right) = \sum_{r=0}^{\infty} \frac{B_{2r}\, x^{2r}}{(2r)!}$$

The calculation of B_{2r} was the output of arguably the first "computer program", by Ada Lovelace and Charles Babbage's "adding machine".

Implications of Euler-Maclaurin

If $f \in C^{\infty}[a,b]$ and periodic with $f^{(j)}(a) = f^{(j)}(b)$ (think Fourier series) then then error $|I - T_n|$ decays superalgebraically as $n \to \infty$.

Def: $\epsilon_n \to 0$ superalgebraically if

$$\lim_{n\to\infty} \frac{\epsilon_n}{h^{pn}} = 0 \quad \text{for any } p > 0.$$

Meaning $\epsilon_n \to 0$ faster than any power of h.

Ex: Show demo for (if time)

$$\int_0^{2\pi} \cos mx \, dx \quad , \quad J_0(x) = \frac{1}{\pi}\int_0^{\pi} e^{ix\cos\theta}$$

For this reason, the trapezoidal rule is very important in various numerical methods.

2nd If time: the E-M formula allows for the application of Richardson extrapolation

Legendre Polynomials are the set of polynomials which are orthogonal on the interval $[-1,1]$.

Gram-Schmidt rewritten slightly:

$$\hat{P}_0 = \frac{1}{\sqrt{\int 1^2 dx}}$$

For $n = 1, 2, \ldots$

① $$P_n(x) = \underbrace{x\,\hat{P}_{n-1}(x)}_{\text{increments degree by one}} - \sum_{j=0}^{n-1} \left(x\hat{P}_{n-1}(x), \hat{P}_j(x)\right)\hat{P}_j(x)$$

And $$\left(x\hat{P}_{n-1}(x), \hat{P}_j(x)\right) = \int x\,\hat{P}_{n-1}(x)\,\hat{P}_j(x)\,dx$$

② $$\hat{P}_n(x) = \frac{P_n(x)}{\| P_n(x) \|}$$

<u>But</u> by construction, P_{n-1} is orthogonal to all polynomials of degree $\leq n-2$.

$$\Rightarrow \left(x\hat{P}_{n-1}, \hat{P}_j\right) = \left(\hat{P}_{n-1}, x\hat{P}_j\right) = 0 \quad \text{if } j \leq n-3.$$

$$\Rightarrow P_n(x) = x\,\hat{P}_{n-1}(x) - \left(x\hat{P}_{n-1}, \hat{P}_{n-1}\right)\hat{P}_{n-1} - \left(x\hat{P}_{n-1}, \hat{P}_{n-2}\right)\hat{P}_{n-2}$$

$\Rightarrow$ <u>Three term recurrence</u> $\Rightarrow$ P_n can be calculated using P_{n-1}, P_{n-2}

For Legendre polynomials, this recurrence takes the form:

$$P_{n+1}(x) = \frac{2n+1}{n+1} x P_n(x) - \frac{n}{n+1} P_{n-1}(x)$$

(Just like for Chebyshev polynomials earlier.)

Why do we care about orthogonal polynomials?
It turns out that they are used to calculate the <u>nods</u> for Gaussian Quadratures:

<u>Thm</u>: If $x_1, \dots, x_n$ are the zeros (roots) of $P_n(x)$, the n^{th} orthogonal polynomial on $\frac{[-1,1]}{[a,b]}$, then the formula:

$$\int_a^b f(x) \approx \sum_{j=1}^{n} w_j f(x_j)$$

where

$$w_j = \int_a^b \varphi_j(x)\,dx \qquad \varphi_j(x) = \prod_{l \neq j} \frac{x - x_l}{x_j - x_l}$$

is <u>exact</u> for polynomials of degree $2n-1$ or less.

$\Rightarrow$ Exact for $2n$ linearly independent functions!

Proof

Assume f is a polynomial, $\deg(f) \le 2n-1$.

This implies that $f = q P_n + r$

$$\left.\begin{aligned} \deg(q) &\le n-1 \\ \deg(r) &\le n-1 \end{aligned}\right| \text{ by polynomial long division}$$

If x_j are the roots of P_n, then $f(x_j) = r(x_j)$. Integrating we have:

$$\int_a^b f(x)\,dx = \overbrace{\int_a^b q(x)\,P_n(x)\,dx}^{(q,P_n)=0 \text{ since } \deg(q) \le n-1} + \int_a^b r(x)\,dx$$

$$= 0 + \int_a^b r(x)\,dx$$

And given the choice of weights w_j,

$$\int_a^b r(x)\,dx = \sum w_j r(x_j) = \sum w_j f(x_j). \quad \triangleright$$

To summarize: for an interval $[a,b]$, the n-point Gaussian Quadrature integrates $1, x, \dots x^{2n-1}$ exactly by the rule $\sum w_j f(x_j)$ with x_j the roots of P_n, the degree-n orthogonal polynomial on the interval. w_j can be solved for.

Another Example Chebyshev Polynomials

Chebyshev polynomials are orthogonal on $[-1,1]$ with a weight function $w(x) = \frac{1}{\sqrt{1-x^2}}$:

$$\int_{-1}^{1} T_n(x) T_m(x) \frac{dx}{\sqrt{1-x^2}} = 0 \quad \text{if } n \neq m.$$

What is the analogue of Gaussian Quadrature here:

Let x_j be the roots of $T_n(x)$.

~~Then we need weights~~ Calculate weights w_j

as

$$w_j = \int_{-1}^{1} \varphi_j(x)\, w(x)\, dx \qquad \varphi_j = \prod_{l \neq j} \frac{x - x_l}{x_j - x_l}$$

then the quadrature rule:

$$\int_{-1}^{1} f(x) \frac{1}{\sqrt{1-x^2}} dx = \sum w_j f(x_j)$$ is exact for

f a polynomial of deg $\leq 2n-1$.

$\Rightarrow$ This procedure works for any positive weight function $w(x)$. ($w(x)$ can be zero at a countable set of points.)