$\boxed{03/24/16}$

Numerical Integration

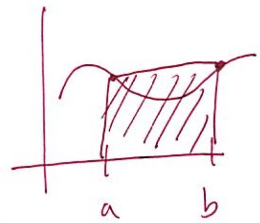
Last time:

- Trapezoidal rule:

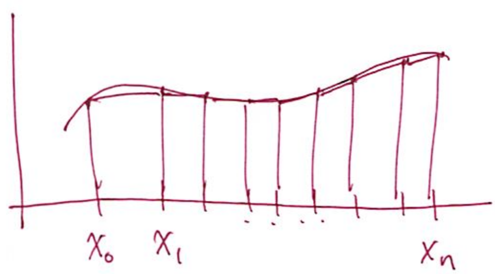
$$\int_a^b f(x)\,dx \approx \underbrace{\frac{b-a}{2}\left(f(a)+f(b)\right)}$$

Mistake last class!

May have had $f(b)-f(a)$ instead of $f(a)+f(b)$



- Composite trapezoidal rule



~~Let $x_j - x_{j-1} = h$~~

~~same size intervals~~

$$\int_{x_0}^{x_n} f(x)\,dx \approx \sum_{j=1}^{n}\left(\frac{x_j - x_{j-1}}{2}\right)\left(f(x_j)+f(x_{j-1})\right)$$

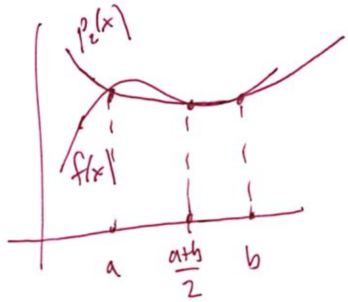
- Special case of Newton-Cotes Formulas

Interpolate f at nodes, integrate the interpolant.

Equal intervals: $x_j - x_{j-1} = h$

$$\Rightarrow \int_{x_0}^{x_n} f(x)\,dx \approx \sum_{j=1}^{n}\frac{h}{2}\left(f(x_j)+f(x_{j-1})\right) = h\sum_{j=0}^{n} f(x_j) - \frac{h}{2}\left(f(x_0)+f(x_n)\right)$$

Ex: 2^{nd} degree interpolant : Simpson's Rule



$$\int_a^b f(x)\,dx \approx \frac{b-a}{6} f(a) + \frac{4(b-a)}{6} f\left(\frac{a+b}{2}\right) + \frac{b-a}{6} f(b)$$

Today Gauss Quadrature.

Definition An n point Gaussian quadrature rule is one of the form

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

that is exact for all polynomials of degree $2n-1$ or less. I.e.

$$\int_a^b p(x)\,dx = \sum_{j=1}^{n} w_j f(x_j) \quad \text{if} \quad \deg(p(x)) \le \underbrace{2n-1}_{2n \text{ function}}$$

Compare with Newton-Cotes formulas: Interp f with p, integrate:

$$\int f(x)\,dx \approx \sum_{j=1}^{n} A_j f(x_j)$$

A_j: n parameters

x_j: usually fixed, (equispaced)

Gaussian rules have 2n parameters : w_j, x_j

How do we find the correct values of the nodes x_j? (Given x_j, the weights could be calculated from the system:

$$\int p_\ell(x) = \sum_j w_j \, p_\ell(x_j) \qquad \text{for } \ell = 0, \dots, n-1.$$

In order to find the nodes x_j, we need to take a diversion...

Orthogonal Polynomials

Def: Two polynomials are orthogonal on $[a,b]$ if

$$\underbrace{(p,q) = \int_a^b p(x)\, q(x)\, dx}_{\text{inner product on } [a,b]} = 0.$$

Orthonormal if orthogonal and $(p,p) = \int_a^b p(x)^2 \, dx = 1$

$(q,q) = 1$

For any interval, ~~as~~ a set ~~&~~ of orthogonal polynomials can be constructed using the Gram-Schmidt Process. (same as in linear algebra)

Ex: Start with $1, x, x^2, \dots$ on $[-1,1]$

Let $p_0(x) = 1$

$$\hat{p}_0(x) = \frac{p_0(x)}{\|p_0\|} = 1 \cdot \frac{1}{\sqrt{\int_{-1}^{1} 1^2\,dx}} = 1 \cdot \frac{1}{\sqrt{2}} = \frac{1}{\sqrt{2}}$$

$$p_1(x) = x - \left(x, \hat{p}_0(x)\right)\hat{p}_0(x)$$

$$= x - \int_{-1}^{1} x \cdot \frac{1}{\sqrt{2}}\,dx \cdot \frac{1}{\sqrt{2}}$$

$$= x - \frac{1}{2}\left[\frac{1}{2}x^2\right]_{-1}^{1} = x - \frac{1}{2}(1-1) = x$$

$$\hat{p}_1(x) = \frac{p_1(x)}{\|p_1\|} = x \cdot \frac{1}{\sqrt{\int_{-1}^{1} x^2\,dx}} = x \cdot \frac{1}{\sqrt{2/3}} = \sqrt{\frac{3}{2}}\,x$$

$$p_2(x) = x^2 - \left(x^2, \hat{p}_0(x)\right)\hat{p}_0(x) - \left(x^2, \hat{p}_1(x)\right)\hat{p}_1(x)$$

$$= x^2 - \int_{-1}^{1} x^2 \frac{1}{\sqrt{2}}\,dx\,\frac{1}{\sqrt{2}} - \int_{-1}^{1} x^2 \sqrt{\frac{3}{2}}\,x\,dx\,\sqrt{\frac{3}{2}}\,x$$

$$= x^2 - \frac{1}{2}\frac{2}{3} - \cancel{\frac{3}{2}x\int_{-1}^{1} x^3\,dx}$$

$$= x^2 - \frac{1}{3}$$

$$\hat{p}_2(x) = \frac{p_2(x)}{\|p_2\|} \quad \dots$$

Up to constant scaling factors, $p_0, p_1, \dots$ are called Legendre Polynomials.

Legendre Polynomials are the set of polynomials ~~wit~~ 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) $$\hat{P}_n(x) = \frac{P_n(x)}{\| P_n(x) \|}$$

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

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

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

$\Rightarrow$ Three term recurrence $\Rightarrow$ 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, $\deg(f) \leq 2n-1$.

This implies that $f = q P_n + r$

$$\left.\begin{array}{l} \deg(q) \leq n-1 \\ \deg(r) \leq n-1 \end{array}\right| \text{ by polynomial long division}$$

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

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

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

And given the choice of weights w_j,

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

To summarize: for an interval $[a,b]$, the n-point Gaussian Quadrature integrates $1, x, \ldots x^{2n-1}$ <u>exactly</u> 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 weig~~ 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:

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

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.)

A note on orthogonal polynomials:

The most common orthogonal polynomials are:

$w(x) = 1, \quad [a,b] = [-1,1] \quad \Rightarrow$ Legendre

$w(x) = \frac{1}{\sqrt{1-x^2}}, \quad [a,b] = [-1,1] \quad \Rightarrow$ Chebyshev

$w(x) = e^{-x}, \quad [a,b] = [0,\infty] \quad \Rightarrow$ Laguerre.

$w(x) = e^{-x^2}, \quad [a,b] = [-\infty,\infty] \quad \Rightarrow$ Hermite

eigenfunctions of the Fourier Transform.

The corresponding quadrature rules are often called:

Gauss-Legendre, Gauss-Laguerre, ...

If an interpolating polynomial is constructed at Chebyshev nodes, integrating this polynomial is called Clenshaw-Curtis Quadrature. This can be done in $O(n \log n)$ operations using the FFT (to come later...)

(Will come back to this when we discuss the FFT).

The Trapezoidal Rule for Periodic Function

Recall: For an arbitrary function, using the composite trapezoidal rule:

$$\int_a^b f(x)\,dx \approx \sum_{j=0}^{n} h f(x_j) - \frac{h}{2}\left(f(x_0) + f(x_n)\right) + \underbrace{O(h^2)}_{\substack{\text{Global} \\ \text{approximate} \\ \text{error}}}$$

$$h = \frac{(b-a)}{n}$$

After much algebra (p244–245), we can explicitly write down the error in the composite trapezoidal rule:

<u>Thm</u> (Euler-Maclaurin ~~The~~ Formula): Let $f \in C^{2n}[a,b]$ and $T_n(f)$ is the composite trapezoidal rule for $\int_a^b f$. Then

$$T_n(f) - \int_a^b f(x)\,dx = \frac{h^2}{12}\left(f'(b) - f'(a)\right) - \frac{h^4}{720}\left(f^{(3)}(b) - f^{(3)}(a)\right)$$

$$+ \frac{h^6}{30240}\left(f^{(5)}(b) - f^{(5)}(a)\right) - \cdots$$

$$+ (-1)^{n-1}\frac{b_{2n}}{(2n)!} h^{2n} f^{(2n)}(\xi) \qquad \xi \in [a,b]$$

$(-1)^{j-1} b_{2j}$ = Bernoulli Numbers

$\Rightarrow$ If f is periodic, $f^{(n)}(b) = f^{(n)}(a)$! Error terms are 0!

If f is infinitely differentiable (think Fourier series), then take $n \to \infty$ in E-M Formula.

The error then goes down faster than any power of h

This is called superalgebraic convergence.