§10 Numerical integration II

Recall: For Newton-Cotes integration, we used polynomial interpolation on equally spaced nodes, and used exact integration of the polynomial:

polynom. approx. of f

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

Newton-Cotes: $n=1 \longrightarrow$ Trapezoidal rule

$n=2 \longrightarrow$ Simpson's rule

With these rules we could integrate $p \in \mathbb{P}_n$ exactly

Main idea behind Gauss quadrature: Allow node locations to change, which gives us additional flexibility / degrees of freedom. Can we do better than Newton-Cotes?

$$\int_a^b f(x)\,dx \approx \sum_{j=0}^{n} w_j\, f(x_j)$$

quadrature nodes

quadrature weights

Generalize formulation

$$\int_a^b w(x)\, f(x)\,dx \approx \sum_{i=0}^{n} w_i\, f(x_i)$$

We assume to-be-determined $x_0, \dots, x_n$ and instead of Lagrange interpolation, let us try Hermite interpolation:

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

$H_k(x_j) = \begin{cases} 1 & k=j \\ 0 & \text{else} \end{cases}$ $\qquad K_k(x_j) = 0$ $\qquad$ for all

$H_k'(x_j) = 0$ $\qquad K_k'(x_j) = \begin{cases} 1 & k=j \\ 0 & \text{else} \end{cases}$ $\qquad k,j \in \{0,\dots,n\}$

$$\int_a^b w(x)\, f(x)\, dx \approx \int_a^b p_{2n+1}(x)\, w(x)\, dx$$

$$= \sum_{k=0}^{n} f(x_k) \underbrace{\int_a^b w(x)\, H_k(x)\, dx}_{W_k} + \sum_{k=0}^{n} f'(x_k) \underbrace{\int_a^b w(x)\, K_k(x)\, dx}_{V_k}$$

We do not want to involve $f'(x_k)$ in the computation, so can we find quadrature nodes $x_0,\dots,x_n$ such that $V_k = 0$, $k=0,\dots,n$?

$$K_k(x) = L_k(x)^2 (x - x_k), \qquad L_k(x) = \prod_{\substack{j=0 \\ j\neq k}}^{n} \frac{x - x_j}{x_k - x_j}$$

$$V_k = \int_a^b w(x)\, L_k(x)^2 (x - x_k)\, dx$$

$$= \int_a^b w(x) \frac{\overbrace{(x-x_0)\cdot \ldots \cdot (x-x_n)}^{\pi_{n+1}(x) \in P_{n+1}}}{\underbrace{\prod_{\substack{j=0 \\ j\neq k}}^{n} (x_k - x_j)}_{C}} L_k(x)\, dx = \frac{1}{C}\int_a^b w(x)\, \underbrace{\pi_{n+1}(x)}_{\in P_{n+1}}\, \underbrace{L_k(x)}_{\in P_n}\, dx$$

__Thus:__ For $V_k = 0$ for all k, we need π_{n+1} to be orthogonal to each $L_k(x)$, and thus to all $p \in P_n$

We know how to do that! In the previous chapter we did compute $\{\underbrace{\varphi_0, \varphi_1, \dots,}_{\text{span } P_n} \varphi_{n+1}\}$ orthogonal basis. We also know that the roots of orthogonal polynomials φ_{n+1} are real and distinct, and in (a,b) $\Longrightarrow$ these roots should be our interpolation nodes (since then $\varphi_{n+1} = C\,\pi_{n+1}$, $C \in \mathbb{R}$)

Simplify W_k's:

$$W_k = \int_a^b w(x)\, H_k(x)\, dx = \qquad H_k(x) = L_k(x)^2 \left(1 - 2L_k'(x_k)(x-x_k)\right)$$

$$= \int_a^b w(x)\, L_k(x)^2\, dx - 2L_k'(x_k) \underbrace{\int_a^b w(x)\, L_k(x)^2 (x-x_k)\, dx}_{V_k = 0}$$

$\Rightarrow$ Gauss quadrature rule:

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

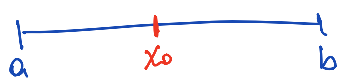
$W_k = \int_a^b w(x)\, L_k(x)^2\, dx$

$x_0, \ldots, x_n$ roots of ortho g. poly.

Construction: (1) Define quadrature points $x_0, \ldots, x_n$ as the $n+1$ roots of the polynomial of degree $n+1$ of a system of orthogonal polynomials on (a,b) with respect to $w(x)$

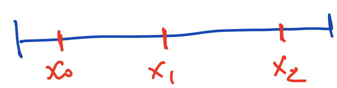
Gauss quadrature points

$w \equiv 1$, $n = 0$



$w \equiv 1$, $n = 1$

$w \equiv 1$, $n = 2$



(2) Calculate Weights $W_k = \int_a^b w(x)\, L_k(x)^2\, dx$

(3) Use Gauss quadrature for $f: [a,b] \to \mathbb{R}$

from (2) from (1)

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

How accurate is this rule:

Hermite interpolation has the error estimate

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

$$M_{2n+2} = \max_{x \in [a,b]} |f^{(2n+2)}(x)|$$

$\Longrightarrow$ Hermite interpolation is <u>exact</u> for $p \in \mathbb{P}_{2n+1}$

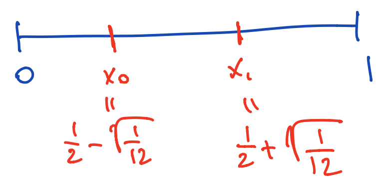
$\Longrightarrow$ Gauss quadrature is exact for polynomials of degree $\leq 2n+1$!

<u>Example:</u> $n = 1$, $w(x) \equiv 1$, interval $(0,1)$

(1) orthogonal polynomials $\{1, x - \frac{1}{2}, \underbrace{x^2 - x + \frac{1}{6}}_{\varphi_2(x)}\}$

roots of φ_2:

$$x_{1,2} = \frac{1}{2} \pm \sqrt{\frac{1}{12}}$$



(2) weights:

$$W_0 = \int_0^1 L_0(x)^2 \, dx = \int_0^1 \left(\frac{x - x_1}{x_0 - x_1}\right)^2 dx = \frac{1}{2}$$

$$W_1 = \frac{1}{2}$$

(3) Use formula: $f : [a,b] \to \mathbb{R}$

$$\int_0^1 f(x)\,dx \approx \frac{1}{2} f\left(\frac{1}{2} - \sqrt{\frac{1}{12}}\right) + \frac{1}{2} f\left(\frac{1}{2} + \sqrt{\frac{1}{12}}\right)$$

exact whenever f is a polynomial of degree $2n+1 = 3$

i.e: $\displaystyle\int_0^1 \underbrace{x^3 - 3x^2 + 7x}_{f(x)} = \frac{1}{2} f\left(\frac{1}{2} - \sqrt{\frac{1}{12}}\right) + \frac{1}{2} f\left(\frac{1}{2} + \sqrt{\frac{1}{12}}\right)$

With Newton-Cotes, 2 evaluations of f is the trapezoidal rule, which is exact for polynomials of degree $\leq n = 1$