§10 Gauss quadrature

Newton-Cotes:

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

polynomial interpolant of f with degree n

weights

nodes

$n=1 \longrightarrow$ trapezoidal rule

$n=2 \longrightarrow$ Simpson's rule

We can integrate polynomials of degree n exactly.

Main idea about Gauss quadrature: Allow nodes $x_0, \dots, x_n$ to change, giving us additional flexibility.

More general:
$$\int_a^b w(x) f(x)\,dx \approx \sum_{j=0}^{n} w_j f(x_j) \qquad w(x) > 0 \text{ for all } x$$

Let's try a Hermite interpolation of f:

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

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

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

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 $V_k = 0$, $k = 0, \dots, n$?

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

$$V_k = \int_a^b w(x)\, L_k(x)^2 (x-x_k)\, dx = \int_a^b w(x) \frac{\overbrace{(x-x_0)\cdot \ldots (x-x_n)}^{\pi_{n+1}}}{\underbrace{\prod_{\substack{j=0\\ j\neq k}}^{n} (x_k - x_j)}_{C}} L_k(x)\, dx$$

$$= \frac{1}{C} \int_a^b w(x)\, \underbrace{\pi_{n+1}(x)}_{\in P_{n+1}}\, \underbrace{L_k(x)}_{\in P_k}\, dx$$

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

We know how to do this — we can construct an orthogonal basis $\{\varphi_0, \varphi_1, \ldots, \varphi_{n+1}\}$, and we can show that the roots of these orthogonal polynomials are all in (a,b) and they are single $\longrightarrow$ thus π_{n+1} should be the $(n+1)$-st orthogonal polynomial and $x_0, \ldots, x_n$ must be the roots of that polynomial.

Simplify W_k's:

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

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

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

Gauss quadrature rule:

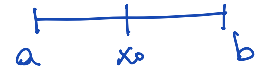
$$\int_a^b w(x) f(x)\, dx \approx \sum_{k=0}^{n} W_k f(x_k)$$

$x_0, \ldots, x_n \ldots$ roots of $(n+1)$ st orthogonal polynomial

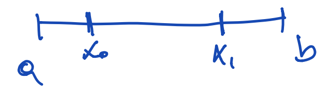
Construction of Gauss quadrature rule:

(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 polyn. w.r. to (a,b) and weight $w(x)$.

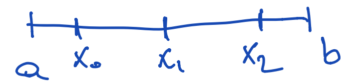
Gauss quad: $w \equiv 1$, $n=0$



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



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



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

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

$$\int_a^b w(x) f(x)\, dx \simeq \sum_{k=0}^{n} \underbrace{W_k}_{\text{from (2)}} f(\underbrace{x_k}_{\text{from (1)}})$$

How accurate is this? Hermite interpolation error has the estimate

$$|f(x) - p_{2n+1}(x)| \le \frac{M_{2n+2}}{(2n+2)!} |\pi_{n+1}(x)|^2$$

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

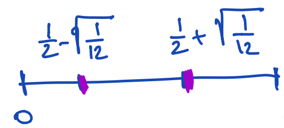
$\longrightarrow$ Hermite interpolation is <u>exact</u> for $p \in P_{2n+1}$

$\longrightarrow$ Gauss quadrature is also exact for polynomials of degree $\le 2n+1$.

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

(i) orthog. poly: $\{1, x - \frac{1}{2}, \underbrace{x^2 - x + \frac{1}{6}}_{\varphi_2(x)}\}$

roots of φ_2: $x_{1,2} = \frac{1}{2} \pm \sqrt{\frac{1}{12}}$



(ii) weights:

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

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

(iii) 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 $\leq 2n+1 = 3$

i.e: $$\int_0^1 \underbrace{x^3 - 3x^2 - 17x}_{f}\,dx = \frac{1}{2} f\left(\frac{1}{2} - \sqrt{\frac{1}{12}}\right) + \frac{1}{2} f\left(\frac{1}{2} + \sqrt{\frac{1}{12}}\right)$$

in comparison, with Newton-Cotes, two evaluations of f is the trapezoidal rule which is only exact for polynomials of degree $\leq n = 1$.