Gauss Quadrature

Idea: Choose the nodes and the weights simultaneously.

One interval:

$$\int_a^b f(x)\,dx = A_0 f(x_0) + A_1 f(x_1)$$

weights : A_0, A_1
nodes : x_0, x_1 ; $n = 1$ $(n+1)$-rule

Coefficients are determined by the usual process:

$$\int_a^b 1\,dx = b - a = A_0 + A_1$$

$$\int_a^b x\,dx = \frac{1}{2}(b^2 - a^2) = A_0 x_0 + A_1 x_1$$

$$\int_a^b x^2\,dx = \frac{1}{3}(b^3 - a^3) = A_0 x_0^2 + A_1 x_1^2$$

. . .

The resulting system is nonlinear!

ORTHOGONAL POLYNOMIALS

Inner product of two polynomials:

$$\langle p, q \rangle = \int_a^b p(x)\, q(x)\, dx$$

DEFINITION (Orthogonality)

Two polynomials are orthogonal on $[a, b]$ if their inner product is zero.

Orthogonality: $\langle p, q \rangle = 0$

orthonormal: $\langle p, p \rangle = 1 = \langle q, q \rangle$

GRAM-SCHMIDT PROCEDURE:

Norm: $\| q(x) \| = \left[\int_a^b (q(x))^2 dx \right]^{1/2}$

Idea: Transform a basis to an orthogonal one:

$$\{ 1, x, x^2, \dots, x^k, \dots \}$$

$$\xrightarrow{G-S} \{ q_0, q_1, \dots, q^k, \dots \} \text{ ortho-normal}$$

$$q_0 = \frac{1}{\| 1 \|} = \frac{1}{\left[\int_a^b 1^2 \, dx \right]^{1/2}} = \frac{1}{\sqrt{b-a}}$$

for $j = 1, 2, \ldots$

$$\tilde{q}_j(x) = x q_{j-1}(x) - \sum_{i=0}^{j-1} \underline{\langle x q_{j-1}(x), q_i(x) \rangle} \, q_i(x)$$

$$q_j(x) = \tilde{q}_j(x) / \| \tilde{q}_j(x) \|$$

This new basis is orthonormal!

Observation:

$q_{j-1}(x)$ is orthogonal to all polynomials of degree $j-2$ or less.

Thus:

$$\underline{\langle x q_{j-1}(x), q_i(x) \rangle} =$$

$$\langle q_{j-1}(x), x q_i(x) \rangle = 0, \quad i \leq j-3$$

$$\Rightarrow \quad \tilde{q}_j(x) = x\,q_{j-1}(x) - \langle x q_{j-1}(x), q_{j-1}(x)\rangle\, q_{j-1}(x) - \langle x q_{j-1}(x), q_{j-2}(x)\rangle\, q_{j-2}(x)$$

Three-term recurrence rule!

$$\begin{aligned}
\langle \tilde{q}_j(x), q_{j-1}(x)\rangle &= \langle x q_{j-1}(x), q_{j-1}(x)\rangle - \sum_{i=0}^{j-1} \langle x q_{j-1}(x), q_i(x)\rangle \cdot \underbrace{\langle q_i(x), q_{j-1}(x)\rangle}_{\substack{=0,\ \text{except} \\ \text{when } i=j-1 \\ =1}} \\
&= \langle x q_{j-1}(x), q_{j-1}(x)\rangle - \langle x q_{j-1}(x), q_{j-1}(x)\rangle = 0
\end{aligned}$$

GRAM-SCHMIDT WORKS!

THEOREM Let $x_0, x_1, \dots, x_n$ roots of an orthogonal polynomial $q_{n+1}(x)$ on $[a,b]$.

Then
$$\int_a^b f(x)\,dx \simeq \sum_{i=0}^{n} A_i f(x_i),$$

where
$$A_i = \int_a^b \varphi_i(x)\,dx, \quad \varphi_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j},$$

is exact for all polynomials of degree $2n+1$ or less.

<u>Proof</u> Let f be such a polynomial.

Division algorithm:

$$f = q_{n+1} p_n + \underbrace{r_n}_{\text{maximal degree } n}$$

Then
$$f(x_i) = \underbrace{q_{n+1}(x_i)}_{=0} p_n(x_i) + r_n(x_i)$$

$$= r_n(x_i)$$

Integrate:

$$\int_a^b f(x)\,dx = \underbrace{\int_a^b q_{n+1}(x)\,p_n(x)\,dx}_{\langle q_{n+1},\, p_n \rangle \,=\, 0} + \int_a^b r_n(x)\,dx$$

$$= \int_a^b r_n(x)\,dx \quad \text{(can be interpolated)}$$

$$= \sum_{i=0}^{n} A_i\, r_n(x_i) = \sum_{i=0}^{n} A_i\, f(x_i)$$

$\square$

DEFINITION Weighted orthogonal polynomials

$$\langle p, q \rangle_w = \int_a^b p(x)\, q(x)\, w(x)\, dx,$$

where $w(x)$ is a positive weight function.

THEOREM The previous theorem holds for a w-orthogonal polynomial q_{n+1}:

$$A_i = \int_a^b \varphi_i(x)\, w(x)\, dx$$

Error formula : n-point rule (2n-1 degree)

$$\text{error} = \frac{f^{(2n)}(\xi(x))}{(2n!)} \prod_{k=1}^{n} (x - x_k)^2$$

Where does that square come from?

We assume that the derivatives of f are continuous, therefore Hermite interpolation is the natural choice.

EXAMPLE Gauss rule : $[-1,1]$; $n = 1$

Notice : Since we only want the roots, there is no need to normalise.

GS :
$$\tilde{q}_0 = 1$$

$$\tilde{q}_1 = x \cdot 1 - \frac{\langle x, 1 \rangle}{\langle 1, 1 \rangle} \cdot 1$$

$$= x - \left[\left(\int_{-1}^{1} x \, dx \right) \Big/ \left(\int_{-1}^{1} 1 \, dx \right) \right] \cdot 1$$

$$= x$$

$$\tilde{q}_2 = x \cdot x - \frac{\langle x^2, 1\rangle}{\langle 1, 1\rangle} \cdot 1 - \frac{\langle x^2, x\rangle}{\langle x, x\rangle} \cdot x$$

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

Roots : $x = \pm \frac{1}{\sqrt{3}}$

Quadrature :

$$\int_{-1}^{1} f(x)\,dx = A_0 f\left(-\frac{1}{\sqrt{3}}\right) + A_1 f\left(\frac{1}{\sqrt{3}}\right)$$

Now : $\left.\begin{aligned} \int_{-1}^{1} 1\,dx &= 2 = A_0 + A_1 \\ \int_{-1}^{1} x\,dx &= 0 = -\frac{A_0}{\sqrt{3}} + \frac{A_1}{\sqrt{3}} \end{aligned}\right\} A_0 = A_1 = 1$

$$\int_{-1}^{1} x^2\,dx = \frac{2}{3} = 1 \cdot \left(-\frac{1}{\sqrt{3}}\right)^2 + 1 \cdot \left(\frac{1}{\sqrt{3}}\right)^2$$

$$\int_{-1}^{1} x^3\,dx = 0 = 1 \cdot \left(-\frac{1}{\sqrt{3}}\right)^3 + 1 \cdot \left(\frac{1}{\sqrt{3}}\right)^3$$

HURRAH!