Gaussian Quadrature Schemes

Consider an integration scheme of the form:

$$\int_a^b f(x)\,dx = A_0 f(x_0) + A_1 f(x_1) + \cdots + A_n f(x_n) \qquad (1)$$

With Newton-Cotes

a) We set $x_k = a + kh$

b) We find $A_0, A_1, \ldots, A_n$ such that (1) is exact for polynomials with degree $\leq n$.
(n+1 degrees of freedom).

▶ Idea : Treat both x_k and A_k as unknowns and derive a scheme which is exact for polynomials with degree $\leq 2n+1$.

▶ Example : For $n=1$, $a=0$, $b=1$,
integrate $1, x, x^2, x^3$

$$\begin{aligned}
f(x) = 1 &\longrightarrow 1 = A_0 + A_1 \cdot 1 \\
f(x) = x &\longrightarrow 1/2 = A_0 x_0 + A_1 x_1 \\
f(x) = x^2 &\longrightarrow 1/3 = A_0 x_0^2 + A_1 x_1^2 \\
f(x) = x^3 &\longrightarrow 1/4 = A_0 x_0^3 + A_1 x_1^3
\end{aligned}$$

We get a nonlinear system of equations which is hard to solve.

To circumvent the need to deal with nonlinear equations we use the following more general method:

▶ <u>Problem</u> : Let $w(x)$ be a weight function such that
$w(x) > 0, \forall x \in (a,b)$.
Want to find $A_0, A_1, \dots, A_n$ and $x_0, x_1, \dots, x_n$ to approximate

$$\int_a^b f(x) w(x) dx \cong A_0 f_0(x) + A_1 f_1(x_1) + \dots + A_n f(x_n)$$

such that it is exact for $f(x)$ polynomial of degree $\leq 2n+1$.

▶ <u>Solution</u>

<u>Def</u> : Let f, g be two functions. We define the scalar product

$$\langle f | g \rangle = \int_a^b f(x) g(x) w(x) dx$$

We say that $f \perp g \Leftrightarrow \langle f | g \rangle = 0$
Aloso define the norm $\|f\| = \sqrt{\langle f | f \rangle}$.

• 1 Construct a sequence of polynomials

$p_0, p_1, \ldots, p_n, \ldots$

such that they are orthogonal to each other as follows:

$$\begin{cases} p_{-1}(x) = 0, \quad p_0(x) = 1 \\ p_{n+1}(x) = (x - a_n) p_n(x) - b_n p_{n-1}(x) \end{cases}$$

where

$$a_n = \frac{\langle x p_n | p_n \rangle}{\langle p_n | p_n \rangle}, \quad \text{for } n = 0, 1, 2, \ldots$$

$$b_n = \frac{\langle p_n | p_n \rangle}{\langle p_{n-1} | p_{n-1} \rangle}, \quad \text{for } n = 1, 2, 3, \ldots$$

$b_0 = 0$

• 2 We find the gridpoints using the following result

<u>Thm</u>: (Fundamental Theorem of Gaussian Quadrature)

The points $x_0, x_1, \ldots, x_N$ for an N-point Gaussian quadrature formula are the roots of $p_N(x)$!

Thm : (Gauss-Lucas)

$$\boxed{\text{The roots of } p_N(x) \text{ are interlaced between the roots of } p_{N-1}(x)}$$

example : If x_1, x_2 are the roots of $p_2(x)$ and y_1, y_2, y_3 the roots of $p_3(x)$ then

$$a < y_1 < x_1 < y_2 < x_2 < y_3 < b$$

- The roots can therefore be found recursively by binary search.

(If the root $x_k \in [\gamma_k, \delta_k]$, split the interval by half and see which half the root belongs to. Keep splitting!)

- The roots of $p_1(x)$, $p_2(x)$ are easy to find.

$\bullet_3$ Given the gridpoints, we find the weights $A_0, A_1, \dots, A_n$ by observing that

$$\int_a^b p_0(x)\,w(x)\,dx = \int_a^b w(x)\,dx = \|1\|$$

$$\int_a^b p_n(x)\,w(x)\,dx = \int_a^b p_n(x)\,p_0(x)\,w(x)\,dx =$$

$$= \langle p_n | p_0 \rangle = 0 \;!!$$

We apply quadrature equation to the above integrals:

$$\begin{bmatrix} p_0(x_0) & p_0(x_1) & p_0(x_2) & \cdots & p_0(x_n) \\ p_1(x_0) & p_1(x_1) & p_1(x_2) & \cdots & p_1(x_n) \\ p_2(x_0) & p_2(x_1) & p_2(x_2) & \cdots & p_2(x_n) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ p_n(x_0) & p_n(x_1) & p_2(x_n) & \cdots & p_n(x_n) \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ \vdots \\ A_n \end{bmatrix} = \begin{bmatrix} \|1\| \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

We can solve with QR decomposition (or LU pivoted) and find A_k.
A faster way to calculate the weights is the formula

$$\boxed{A_n = \frac{\langle p_{N-1} | p_{N-1} \rangle}{p_{N-1}(x_n)\, p_N'(x_n)}}$$

We verify sanity of calculation by evaluating A_n using one method and testing them on the other method.

<u>Remark</u> : The coefficients a_n, b_n needed to calculate $p_{n+1}(x)$ are evaluated using Gaussian-Quadrature formula over the roots of $p_n(x)$!!
Thus we use one quadrature formula to calculate the next one.
Given a_n, b_n we may evaluate $p_n(x)$ recursively at any point!

<u>Theoretical calculation of a_n, b_n</u>

1) For $w(x) = 1, \forall x \in (-1,1)$

$$p_{n+1}(x) = \frac{2n+1}{n+1} x p_n(x) - \frac{n}{n+1} p_{n-1}(x)$$

(Legendre Polynomials)

2) $w(x) = \dfrac{1}{\sqrt{1-x^2}}$, $\forall x \in (-1,1)$

$p_{n+1}(x) = 2x p_n(x) - p_{n-1}(x)$

(Chebyshev Polynomials)

3) $w(x) = x^a e^{-x}$, $\forall x \in (0,+\infty)$

$$p_{n+1}(x) = \frac{-x+2n+a+1}{n+1} p_n(x) - \frac{n+a}{n+1} p_{n-1}(x)$$

(Laguerre polynomials)

4) $w(x) = e^{-x^2}$, $\forall x \in (0,+\infty)$

$p_{n+1}(x) = 2x p_n(x) - 2n p_{n-1}(x)$

(Hermite polynomials)