Gaussian Quadrature

Newton-Cotes formulas:

- The choice of nodes $x_0, x_1, \ldots, x_n$ was made *a priori*.
- Use values of the function at equally spaced points.
- Once the nodes were fixed, the coefficients were determined, e.g., by integrating the fundamental Lagrange polynomials of degree n.
- These formulas are exact for polynomials of degree $\leq n$.

This approach is convenient when the formulas are combined to form the composite rules, but the restriction may decrease the accuracy of the approximation.

Gaussian quadrature

1. Chooses the points for evaluation in an optimal, rather than pre-fixed or equally-spaced, way.
2. The nodes $x_0, x_1, \ldots, x_n \in [a, b]$ and the coefficients $c_0, c_1, \ldots, c_n$ are chosen to minimize the expected error obtained in the approximation

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i) \tag{34}$$

3. Produce the exact result for the largest class of polynomials, that is, the choice which gives the greatest degree of precision.

The coefficients $c_0, c_1, \ldots, c_n$ are arbitrary, and the nodes $x_0, x_1, \ldots, x_n$ are restricted only in $[a, b]$. These give $2n + 2$ degrees of freedom. Thus we can expect that the quadrature formula of (34) can be discovered that will be exact for polynomials of degree $\leq 2n + 1$.

Suppose we want to determine c_1, c_2, x_1 and x_2 so that

$$\int_{-1}^{1} f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) \tag{35}$$

gives the exact result whenever $f(x)$ is a polynomial of degree $2 \times 2 - 1 = 3$ or less, i.e.,

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3.$$

Since

$$\begin{aligned} & \int (a_0 + a_1 x + a_2 x^2 + a_3 x^3) dx \\ = \; & a_0 \int 1 dx + a_1 \int x dx + a_2 \int x^2 dx + a_3 \int x^3 dx, \end{aligned}$$

this is equivalent to show that (35) gives exact results when $f(x)$ is $1, x, x^2$ and x^3. Hence

$$
\begin{aligned}
c_1 + c_2 &= \int_{-1}^{1} 1 dx = 2, \\
c_1 x_1 + c_2 x_2 &= \int_{-1}^{1} x dx = 0, \\
c_1 x_1^2 + c_2 x_2^2 &= \int_{-1}^{1} x^2 dx = \frac{2}{3}, \\
c_1 x_1^3 + c_2 x_2^3 &= \int_{-1}^{1} x^3 dx = 0.
\end{aligned}
$$

It implies that

$$
c_1 = 1,\ c_2 = 1,\ x_1 = -\frac{\sqrt{3}}{3},\ x_2 = \frac{\sqrt{3}}{3}
$$

which gives

$$
\int_{-1}^{1} f(x)dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right).
$$

Definition

1. In a inner-product space, we say f is orthogonal to g, and write $f \perp g$ if $\langle f, g\rangle = 0$.
2. We write $f \perp G$ if $f \perp g$ for all $g \in G$.
3. We say that a finite or infinite sequence of vectors $f_1, f_2, \ldots$ in an inner-product space is orthogonal if $\langle f_i, f_j\rangle = 0$ for all $i \neq j$, and orthonormal if $\langle f_i, f_j\rangle = \delta_{ij}$.

The space of continuous functions on $[a, b]$ with inner-product defined as

$$\langle f, g\rangle = \int_a^b f(x)g(x)\,dx, \tag{36}$$

is an inner-product space.

Definition

$\{\phi_0, \phi_1, \ldots, \phi_n\}$, where $\phi_i \in C[a,b]$ for all $i = 0, 1, \ldots, n$, is said to be an orthogonal set of functions if

$$\langle \phi_i, \phi_j \rangle = \int_a^b \phi_i(x)\phi_j(x)\,dx = \begin{cases} 0, & \text{when } i \neq j, \\ \alpha_i > 0, & \text{when } i = j. \end{cases}$$

If, in addition, $\alpha_i = 1$ for all i, then the set is said to be orthonormal.

Theorem

The set of polynomials $\{p_0, p_1, \ldots, p_n\}$ defined as follows is orthogonal:

$$p_n(x) = (x - a_n)p_{n-1}(x) - b_n p_{n-2}(x) \qquad (n \geq 2)$$

with $p_0(x) = 1$, $p_1(x) = x - a_1$, and

$$a_n = \frac{\langle x p_{n-1}, p_{n-1} \rangle}{\langle p_{n-1}, p_{n-1} \rangle}, \qquad b_n = \frac{\langle x p_{n-1}, p_{n-2} \rangle}{\langle p_{n-2}, p_{n-2} \rangle}.$$

Proof: It is clear from the formulation that each p_n is a monic polynomial of degree n and is therefore not zero. Hence, the denominators in a_n and b_n are not zero. Now we prove the theorem by induction on n that $\langle p_n, p_i \rangle = 0$ for $i = 0, 1, \ldots, n-1$.
For $n = 1$, it can be shown directly from the definition that

$$\begin{aligned} \langle p_1, p_0 \rangle &= \langle (x - a_1) p_0, p_0 \rangle \\ &= \langle x p_0, p_0 \rangle - a_1 \langle p_0, p_0 \rangle \\ &= \langle x p_0, p_0 \rangle - \frac{\langle x p_0, p_0 \rangle}{\langle p_0, p_0 \rangle} \langle p_0, p_0 \rangle = 0. \end{aligned}$$

Now suppose that the assertion is true for an index $n-1$, where $n \geq 2$. That is

$$\langle p_{n-1}, p_i \rangle = 0, \qquad i = 0, 1, \ldots, n-2, \quad n \geq 2.$$

Now we can verify that

$$
\begin{aligned}
\langle p_n, p_{n-1}\rangle &= \langle (x-a_n)p_{n-1} - b_n p_{n-2}, p_{n-1}\rangle \\
&= \langle xp_{n-1}, p_{n-1}\rangle - a_n\langle p_{n-1}, p_{n-1}\rangle - b_n\langle p_{n-2}, p_{n-1}\rangle \\
&= \langle xp_{n-1}, p_{n-1}\rangle - \frac{\langle xp_{n-1}, p_{n-1}\rangle}{\langle p_{n-1}, p_{n-1}\rangle}\langle p_{n-1}, p_{n-1}\rangle \\
&= 0, \\
\langle p_n, p_{n-2}\rangle &= \langle (x-a_n)p_{n-1} - b_n p_{n-2}, p_{n-2}\rangle \\
&= \langle xp_{n-1}, p_{n-2}\rangle - a_n\langle p_{n-1}, p_{n-2}\rangle - b_n\langle p_{n-2}, p_{n-2}\rangle \\
&= \langle xp_{n-1}, p_{n-2}\rangle - \frac{\langle xp_{n-1}, p_{n-2}\rangle}{\langle p_{n-2}, p_{n-2}\rangle}\langle p_{n-2}, p_{n-2}\rangle \\
&= 0,
\end{aligned}
$$

and, for $i = 1, \ldots, n-3$,

$$\begin{aligned}
\langle p_n, p_i \rangle &= \langle (x - a_n) p_{n-1} - b_n p_{n-2}, p_i \rangle \\
&= \langle x p_{n-1}, p_i \rangle - a_n \langle p_{n-1}, p_i \rangle - b_n \langle p_{n-2}, p_i \rangle \\
&= \langle x p_{n-1}, p_i \rangle \\
&= \langle p_{n-1}, x p_i \rangle \\
&= \langle p_{n-1}, x p_i - a_{i+1} p_i - b_{i+1} p_{i-1} + a_{i+1} p_i + b_{i+1} p_{i-1} \rangle \\
&= \langle p_{n-1}, p_{i+1} + a_{i+1} p_i + b_{i+1} p_{i-1} \rangle \\
&= \langle p_{n-1}, p_{i+1} \rangle + a_{i+1} \langle p_{n-1}, p_i \rangle + b_{i+1} \langle p_{n-1}, p_{i-1} \rangle \\
&= 0.
\end{aligned}$$

Finally, when $i = 0$,

$$\begin{aligned}
\langle p_n, p_0 \rangle &= \langle (x - a_n) p_{n-1} - b_n p_{n-2}, p_0 \rangle \\
&= \langle x p_{n-1}, p_0 \rangle = \langle p_{n-1}, x p_0 \rangle = \langle p_{n-1}, p_1 + a_1 p_0 \rangle = 0.
\end{aligned}$$

Hence the theorem is proved.

Corollary

For any $n > 0$, *the set of polynomials* $\{p_0, p_1, \dots, p_n\}$ *given in the previous theorem is linearly independent and*

$$\langle q, p_n \rangle = \int_a^b q(x) p_n(x)\, dx = 0$$

for any polynomial $q(x)$ *with* $\deg(q(x)) < n$.

Proof: Suppose $\alpha_0, \alpha_1, \dots, \alpha_n$ are real numbers such that

$$P(x) = \alpha_0 p_0(x) + \alpha_1 p_1(x) + \cdots + \alpha_n p_n(x) = 0.$$

This means that the coefficients of the terms $1, x, x^2, \dots x^n$ are all zero. Since $\deg(p_j) = j$ and $\alpha_n p_n$ is the only term in $P(x)$ which contains the x^n term, this implies $\alpha_n = 0$. Hence $P(x)$ can be reduced to

$$P(x) = \sum_{j=0}^{n-1} \alpha_j p_j(x) = 0.$$

Similarly, we have $\alpha_{n-1} = 0, \alpha_{n-2} = 0, \ldots, \alpha_0 = 0$. Therefore, $\{p_0, p_1, \ldots, p_n\}$ is linearly independent.
Suppose $\deg(q) = k < n$. Write

$$q(x) = a_0 p_0(x) + a_1 p_1(x) + \cdots + a_k p_k(x) = \sum_{j=0}^{k} a_j p_j(x),$$

for some real numbers $a_0, a_1, \ldots, a_k$. Then

$$\begin{aligned} \langle q, p_n \rangle &= \int_a^b q(x) p_n(x) w(x)\, dx \\ &= \int_a^b \left(\sum_{j=0}^{k} a_j p_j(x) \right) p_n(x) w(x)\, dx \\ &= \sum_{j=0}^{k} \int_a^b p_j(x) p_n(x) w(x)\, dx = 0. \end{aligned}$$

Let Π_n denote the set of polynomials of degree at most n, that is,

$$\Pi_n = \{p(x) \,|\, p(x) \text{ is a polynomial and } \deg(p) \leq n\}.$$

Definition

Let $f(x)$ be any nonzero continuous function. We say f is orthogonal to Π_n, and denote $f \perp \Pi_n$, if

$$\langle f, p \rangle = \int_a^b f(x)p(x)\, dx = 0,$$

for any $p(x) \in \Pi_n$.

Theorem

Let $q(x)$ be any nonzero polynomial of degree $n+1$, and $q(x) \perp \Pi_n$. If $x_0, x_1, \ldots, x_n$ are the roots of $q(x)$ in $[a, b]$, and

$$c_i = \int_a^b \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} \, dx,$$

then

$$\int_a^b p(x) \, dx = \sum_{i=0}^{n} c_i p(x_i), \quad \textit{for any} \;\; p \in \Pi_{2n+1}.$$

That is, the quadrature rule is exact for any polynomial of degree $\leq 2n+1$.

Proof: For any polynomial $p \in \Pi_{2n+1}$, we can write

$$p(x) = q(x)t(x) + r(x),$$

where $t(x), r(x) \in \Pi_n$. Since $x_0, x_1, \ldots, x_n$ are roots of $q(x)$, we have

$$p(x_i) = q(x_i)t(x_i) + r(x_i) = r(x_i), \qquad i = 0, 1, \ldots, n.$$

By assumption, $q \perp \Pi_n$, we have

$$\langle q, t \rangle = \int_a^b q(x)t(x)\, dx = 0.$$

Since $r(x) \in \Pi_n$, it can be expressed exactly in the Lagrange form

$$r(x) = \sum_{i=0}^{n} r(x_i) \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}.$$

Hence

$$
\begin{aligned}
\int_a^b p(x)\,dx &= \int_a^b q(x)t(x)\,dx + \int_a^b r(x)\,dx \\
&= \int_a^b r(x)\,dx = \int_a^b \sum_{i=0}^{n} r(x_i) \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}\,dx \\
&= \sum_{i=0}^{n} r(x_i) \int_a^b \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}\,dx \\
&= \sum_{i=0}^{n} p(x_i) \int_a^b \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}\,dx \\
&= \sum_{i=0}^{n} c_i p(x_i).
\end{aligned}
$$

If the interval $[a, b]$ is $[-1, 1]$, then we can obtain a set of orthogonal polynomials called the Lengendre polynomials. The first few Lengendre polynomials are

$$
\begin{aligned}
p_0(x) &= 1 \\
p_1(x) &= x \\
p_2(x) &= x^2 - \frac{1}{3} \\
p_3(x) &= x^3 - \frac{3}{5}x \\
p_4(x) &= x^4 - \frac{6}{7}x^2 + \frac{3}{35} \\
p_5(x) &= x^5 - \frac{10}{9}x^3 + \frac{5}{21}x
\end{aligned}
$$

- For a given integer n, the Lengendre polynomial p_{n+1} is a monic polynomial of degree $n+1$ and is orthogonal to the set of first n Lengendre polynomials $\{p_0, p_1, \ldots, p_n\}$.
- By theorem, $\{p_0, p_1, \ldots, p_n\}$ is linearly independent, and, hence, is a basis for the vector space Π_n. This implies that $p_{n+1} \perp \Pi_n$.

Theorem

Suppose that $x_0, x_1, \ldots, x_n$ are the roots of the $(n+1)$-st Lengendre polynomial p_{n+1}, and that for each $i = 0, 1, \ldots, n$,

$$c_i = \int_{-1}^{1} \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}\, dx.$$

If $f(x)$ is any polynomial of degree $\leq 2n+1$, then

$$\int_{-1}^{1} f(x)\, dx = \sum_{i=0}^{n} c_i f(x_i).$$

Gaussian Quadrature Rule

For a given function $f(x) \in C[-1,1]$ and integer n,

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i), \tag{37}$$

where $x_0, x_1, \ldots, x_n$ are the roots of the $(n+1)$-st Lengendre polynomial p_{n+1}, and

$$c_i = \int_{-1}^{1} \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}\,dx. \qquad i = 0, 1, \ldots, n.$$

n	x_i	c_i
0	$x_0 = 0$	$c_0 = 2$
1	$x_0 = -0.5773502692$ $x_1 = 0.5773502692$	$c_0 = c_1 = 1$
2	$x_0 = -0.7745966692$ $x_1 = 0$ $x_2 = 0.7745966692$	$c_0 = \frac{5}{9}$ $c_1 = \frac{8}{9}$ $c_2 = \frac{5}{9}$
3	$x_0 = -0.8611363116$ $x_1 = -0.3399810436$ $x_2 = 0.3399810436$ $x_3 = 0.8611363116$	$c_0 = 0.3478548451$ $c_1 = 0.6521451549$ $c_2 = 0.6521451549$ $c_3 = 0.3478548451$
4	$x_0 = -0.9061798459$ $x_1 = -0.5384693101$ $x_2 = 0$ $x_3 = 0.5384693101$ $x_4 = 0.9061798459$	$c_0 = 0.2369268851$ $c_1 = 0.4786286705$ $c_2 = \frac{128}{225} = 0.568888889$ $c_3 = 0.4786286705$ $c_4 = 0.2369268851$