Num. Integration - Quadrature

Basic Problem – Approximation of integrals

We will investigate methods for computing an approximation to the definite integral:

$$I(f) \equiv \int_a^b f(x)dx.$$

The obvious generic approach is to approximate the integrand $f(x)$ on the interval $[a, b]$ by a function that can be integrated exactly (such as a polynomial) and then take the integral of the approximating function to be an approximation to $I(f)$.

Interpolatory Rules

When an interpolating polynomial, $P_n(x)$,is used the corresponding approximation $I(P_n(x))$ is called an interpolatory rule, Consider writing $P_n(x)$ in Lagrange form,

$$P_n(x) = \sum_{i=0}^{n} f(x_i) l_i(x),$$

where $l_i(x)$ is defined by

$$l_i(x) = \prod_{j=0, j \neq i}^{n} \left(\frac{x - x_j}{x_i - x_j} \right).$$

We then have

$$\begin{aligned} \int_a^b P_n(x)dx &= \int_a^b \sum_{i=0}^{n} f(x_i) l_i(x) dx \\ &= \sum_{i=0}^{n} f(x_i) \int_a^b l_i(x) dx \equiv \sum_{i=0}^{n} \omega_i f(x_i). \end{aligned}$$

Observations

- The 'weights' (the ω_i's) depend only on the interval (the value of a and b) and on the x_i's. In particular these weights are independent of the integrand.
- The interpolatory rules then approximate $I(f)$ by a linear combination of sampled integrand evaluations.
- If $a = x_0 < x_1 < \cdots x_n = b$ are equally spaced the corresponding interpolatory rule is called a Newton-Coates quadrature rule.

Errors in Interpolatory Rules

The error associated with an interpolatory rule is $E(f) = I(f) - I(P_n)$ and satisfies,

$$\begin{aligned} E(f) &= \int_a^b f(x)dx - \int_a^b P_n(x)dx = \int_a^b [f(x) - P_n(x)]dx, \\ &= \int_a^b E_n(x)dx, \end{aligned}$$

where $E_n(x)$ is the error in polynomial interpolation and satisfies,

$$\begin{aligned} E_n(x) &= (x - x_0)(x - x_1) \cdots (x - x_n) f[x_0 x_1 \cdots x_n x], \\ &= \Pi_n(x) f[x_0 x_1 \cdots x_n x]. \end{aligned}$$

In some special cases we can simplify this expression to obtain estimates and/or more insight into the behaviour of the error.

Error Analysis - Special Cases

- First special case – If $\Pi_n(x)$ is of one sign (on $[a, b]$) then the Mean Value Theorem for Integrals implies,

$$
\begin{aligned}
E(f) &= \int_a^b f[x_0 x_1 \cdots x_n x] \Pi_n(x) dx, \\
&= f[x_0 x_1 \cdots x_n \xi] \int_a^b \Pi_n(x) dx,
\end{aligned}
$$

for some $\xi \in [a, b]$. Also since $f[x_0 x_1 \cdots x_n \xi] = \frac{f^{n+1}(\eta)}{(n+1)!}$ for some $\eta \in (a, b)$, we have shown that if $\Pi_n(x)$ is of one sign then,

$$
\boxed{E(f) = \frac{1}{(n+1)!} f^{n+1}(\eta) \int_a^b \Pi_n(x) dx}
$$

Error Analysis - Special Cases

Second special case – If $\int_a^b \Pi_n(x)dx = 0$ we have, for arbitrary x_{n+1},

$$f[x_0 x_1 \cdots x_n x] = f[x_0 x_1 \cdots x_n x_{n+1}] + f[x_0 x_1 \cdots x_{n+1} x](x - x_{n+1}),$$

and therefore,

$$\begin{aligned} E(F) &= \int_a^b f[x_0 x_1 \cdots x_n x]\Pi_n(x)dx, \\ &= \int_a^b f[x_0 x_1 \cdots x_{n+1}]\Pi_n(x)dx + \int_a^b f[x_0 x_1 \cdots x_{n+1} x]\Pi_{n+1}(x)dx, \\ &= \int_a^b f[x_0 x_1 \cdots x_{n+1} x]\Pi_{n+1}(x)dx. \end{aligned}$$

As a result, if $\int_a^b \Pi_n(x)dx = 0$ and we can choose x_{n+1} so that $\Pi_{n+1}(x)$ is of one sign, then using a similar argument as for the first special case, it follows that, if $\int_a^b \Pi_n(x)dx = 0$ and $\Pi_{n+1}(x)$ is of one sign,

$$\boxed{E(f) = \frac{1}{(n+2)!} f^{n+2}(\eta) \int_a^b \Pi_{n+1}(x)dx}$$

Examples of Interp. Rules

Trapezoidal Rule (an example of the first special case):

$$T(f) \equiv \int_a^b P_1(x)dx,$$

where $x_0 = a$ and $x_1 = b$. We then have,

$$P_1(x) = l_0(x)f_0 + l_1(x)f_1 = \frac{x - x_1}{x_0 - x_1}f_0 + \frac{x - x_0}{x_1 - x_0}f_1.$$

Therefore we have

$$\begin{aligned} T(f) &= \int_a^b \frac{x-b}{a-b}dx f(a) + \int_a^b \frac{x-a}{b-a}dx f(b), \\ &= \left(\frac{b-a}{2}\right) f(a) + \left(\frac{b-a}{2}\right) f(b) = \left(\frac{b-a}{2}\right)[f(a) + f(b)]. \end{aligned}$$

Examples of Interp. Rules

We also have that $\Pi_1(x) = (x-a)(x-b)$ is negative for $x \in [a,b]$ and $\int_a^b \Pi_1(x)dx = -\frac{(b-a)^3}{6}$. We therefore have satisfied the conditions of the first special case and this implies,

$$\boxed{T(f) = (\tfrac{b-a}{2})[f(a)+f(b)], \quad E^T(f) = \frac{-f^{''}(\eta)}{12}(b-a)^3.}$$

Simpsons Rule (an example of the second special case):

$$S(f) \equiv \int_a^b P_2(x)dx,$$

with $x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b$.

Simpsons Rule

Exercise: Using

$$P_2(x) = l_0(x)f(a) + l_1(x)f\left(\frac{a+b}{2}\right) + l_2(x)f(b),$$

where

$$\begin{aligned} l_0(x) &= \frac{(x-\frac{a+b}{2})(x-b)}{(a-\frac{a+b}{2})(a-b)}, \;\; l_1(x) = \frac{(x-a)(x-b)}{(\frac{a+b}{2}-a)(\frac{a+b}{2}-b)}, \\ l_2(x) &= \frac{(x-a)(x-\frac{a+b}{2})}{(b-a)(b-\frac{a+b}{2})}. \end{aligned}$$

Simplify and verify (after some tedious algebra) that,

$$\begin{aligned} S(f) &= [\int_a^b l_0(x)dx]f(a) + [\int_a^b l_1(x)dx]f(\frac{a+b}{2}) + [\int_a^b l_2(x)dx]f(b), \\ &\vdots \qquad \vdots \\ &= \left(\frac{b-a}{6}\right)\left[f(a) + 4f(\frac{a+b}{2}) + f(b)\right]. \end{aligned}$$

Simpsons Rule (cont)

Note that for $x \in [a, b]$, $\Pi_2(x)$ is antisymetric about $\frac{a+b}{2}$ and this implies $\int_a^b \Pi_2(x)dx = 0$. Furthermore by choosing $x_3 = \frac{a+b}{2}$ we have

$$\Pi_3(x) = (x-a)(x-\frac{a+b}{2})^2(x-b),$$

is of one sign and this implies,

$$E^S(f) = I(f) - S(f) = \frac{1}{4!}f^4(\eta)\int_a^b \Pi_3(x)dx.$$

But $\int_a^b \Pi_3(x)dx = -\frac{4}{15}(\frac{b-a}{2})^5$ so we have,

$$\boxed{S(f) = (\frac{b-a}{6})[f(a) + 4f(\frac{a+b}{2}) + f(b)]} \quad \boxed{E^S(f) = \frac{-f^4(\eta)}{90}(\frac{b-a}{2})^5}$$

Gaussian Quadrature

Recall that the error for interp. rules satisfies,
$E(f) = \int_a^b f[x_0 x_1 \cdots x_n x] \Pi_n(x) dx$, and if $\int_a^b \Pi_n(x) dx = 0$ we have,

$$E(f) = \int_a^b f[x_0 x_1 \cdots x_{n+1} x] \Pi_{n+1}(x) dx,$$

for <u>any</u> x_{n+1}. Now if $\int_a^b \Pi_{n+1}(x) = 0$ as well we can show similarly,

$$E(f) = \int_a^b f[x_0, x_1, \cdots x_{n+2}, x] \Pi_{n+2}(x) dx.$$

In general if we let $q_0(x) \equiv 1$ and $q_i(x) \equiv (x - x_{n+1}) \cdots (x - x_{n+i})$ for $i = 1, 2, \cdots (m-1)$. We can then show that if $\int_a^b \Pi_n(x) q_i(x) dx = 0$, for $i = 0, 1, \cdots (m-1)$ then,

$$E(f) = \int_a^b f[x_0 x_1 \cdots x_{n+m} x] \Pi_{n+m}(x) dx.$$

Gaussian Quadrature (cont)

The key idea of GQ is to choose the interpolation points, ($x_0, x_1, \cdots x_n$) such that $\int_a^b \Pi_n(x)q(x)dx = 0$ for all polynomials, $q(x)$, of degree at most n. In particular for the choice $q(x) = q_i(x)$ for $i = 0, 1, \cdots n$ we have $\int_a^b \Pi_n(x)q_i(x)dx = 0$ and,

$$E(f) = \int_a^b f[x_0 x_1 \cdots x_{2n+1} x]\Pi_{2n+1}(x)dx.$$

To ensure that $\Pi_{2n+1}(x)$ is of one sign for $x \in [a\ b]$ we can choose $x_{n+i+1} = x_i$ for $i = 0, 1, \cdots n$ and we then have $\Pi_{2n+1}(x) = \Pi_n^2(x)$,

$$E(f) = f[x_0 x_1 \cdots x_{2n+1}\xi] \int_a^b \Pi_n^2(x)dx = \frac{1}{(2n+2)!} f^{2n+2}(\eta) \int_a^b \Pi_n^2(x)dx.$$

Note that these rules will be exact for all polynomials of degree at most $2n+1$ since $f^{2n+2}(\eta) \equiv 0$.

GQ – Orthoganal Polynomials

How do we choose the x_i's to ensure that $\int_a^b \Pi_n(x) q(x) dx = 0$ for all polynomials, $q(x)$ of degree at most n ? This question leads to the study of orthogonal polynomials.

- Definition: The set of polynomials $\{r_0(x), r_1(x), \cdots r_k(x)\}$ is orthogonal on $[-1, 1]$ iff the following two conditions are satisfied:
  - $\int_{-1}^1 r_i(x) r_j(x) dx = 0,$ for $i \neq j$,
  - The degree of $r_i(x)$ is i for $i = 0, 1, \cdots k$.

Properties

- Properties of orthogonal polynomials:
  - Any polynomial $q_s(x)$ of degree $s \leq k$ can be expressed as.

$$q_s(x) = \sum_{j=0}^{s} c_j r_j(x).$$

  - $r_k(x)$ is orthogonal to all polynomials of degree less than k. That is, $\int_{-1}^{1} r_k(x) q_s(x) dx = 0$ for $s < k$. (This follows from the previous property.)
  - $r_k(x)$ has k simple zeros all in the interval $[-1, 1]$.

Proof (last property)

For $r_k(x)$, let $\{\mu_1, \mu_2, \cdots \mu_m\}$ be the set of points in $[-1, 1]$ where $r_k(x)$ changes sign. It is clear that each μ_j is a zero of $r_k(x)$ and all simple zeros of $r_k(x)$ in $[-1, 1]$ must be in this set. We then have $m \leq k$ as the maximum number of zeros of a polynomial of degree k is k. Assume $m < k$. We then have,

$$\hat{q}_m(x) \equiv \prod_{i=1}^{m}(x - \mu_i),$$

is a polynomial of degree $m < k$ that changes sign at each μ_i and,

$$\int_{-1}^{1} \hat{q}_m(x) r_k(x) dx = 0.$$

But $\hat{q}_m(x)$ and $r_k(x)$ have the same sign for all x in $[-1, 1]$ (they change sign at the same locations). This implies a contradiction (the integrand is of one sign but the integral is zero)– our assumption must be false. We must therefore have $m = k$.

3-Term Recurrence

The $r_k(x)$ also satisfy,

$$r_{s+1}(x) = a_s(x - b_s)r_s(x) - c_s r_{s-1}(x),$$

for $s = 1, 2, \cdots k$, where the a_s are normalization constants, $r_{-1}(x) = 0$, and if $t_s = \int_{-1}^{1} r_s^2(x)dx$ then,

$$b_s = \frac{1}{t_s}\int_{-1}^{1} x r_s^2(x)dx, \quad c_s = \frac{a_s t_s}{a_{s-1}t_{s-1}}.$$

For example, we obtain the classical Legendre polynomials if we normalise so $r_s(-1) = 1$. This leads to,

$$a_s = \frac{2s+1}{s+1}, \;\; b_s = 0, \;\; c_s = \frac{s}{s+1}.$$