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,

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

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

$$l_0(x) = \frac{(x-\frac{a+b}{2})(x-b)}{(a-\frac{a+b}{2})(a-b)}, \quad l_1(x) = \frac{(x-a)(x-b)}{(\frac{a+b}{2}-a)(\frac{a+b}{2}-b)},$$

$$l_2(x) = \frac{(x-a)(x-\frac{a+b}{2})}{(b-a)(b-\frac{a+b}{2})}.$$

Simplify and verify (after some tedious algebra) that,

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

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,

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

Orthogonal Polys on $[a, b]$

- To transform orthogonal polynomials defined on $[-1, 1]$ to $[a, b]$ consider the linear mapping from $[-1, 1] \rightarrow [a, b]$ defined by $x = \frac{b-a}{2} y + \frac{a+b}{2}$. The inverse mapping is $y = \frac{1}{b-a}[2x - b - a]$ and from calculus we know,

$$\int_a^b g(x) dx = (\frac{b-a}{2}) \int_{-1}^1 g(\frac{b-a}{2} y + \frac{a+b}{2}) dy.$$

  This relationship, combined with the properties of Legendre polynomials give a prescription for the choice of the x_i's for GQ: For $i = 0, 1, \cdots n$, set y_i to the i^{th} zero of the Legendre Polynomial, $r_{n+1}(y)$. With this choice we note that $\prod_{j=0}^n (y - y_j) = K \; r_{n+1}(y)$ for some $K \neq 0$.

Choice of the x_i's for GQ

Then with the choice $x_i = \frac{b-a}{2} y_i + \frac{b+a}{2}$ we have,

$$\begin{aligned}
\Pi_n(x) &= \Pi_n(\frac{b-a}{2}y+\frac{a+b}{2}) \;= \prod_{j=0}^{n}(\frac{b-a}{2}y + \frac{a+b}{2} - x_j) \\
&= \prod_{j=0}^{n}(\frac{b-a}{2}y + \frac{a+b}{2} - (\frac{b-a}{2}y_j + \frac{a+b}{2})) \\
&= \prod_{j=0}^{n}\left[\frac{b-a}{2}(y - y_j)\right] \;= (\frac{b-a}{2})^{n+1}\prod_{j=0}^{n}(y - y_j) \\
&= (\frac{b-a}{2})^{n+1} K \; r_{n+1}(y).
\end{aligned}$$

Choice of the x_i's (cont)

Therefore for any polynomial, $q(x)$ of degree at most n,

$$
\begin{aligned}
&\int_a^b \Pi_n(x) q(x) dx \\
&= \quad (\frac{b-a}{2}) \int_{-1}^{1} \Pi_n(x) q(\frac{b-a}{2}y + \frac{b+a}{2}) dy, \\
&= \quad (\frac{b-a}{2}) \int_{-1}^{1} \Pi_n(x) \hat{q}(y) dy, \\
&= \quad (\frac{b-a}{2})^{n+2} K \int_{-1}^{1} r_{n+1}(y) \hat{q}(y) dy \quad = \quad 0.
\end{aligned}
$$

since $\hat{q}(y)$ is a polynomial of degree at most n.

That is with the x_i's chosen as the 'transformed zeros' of the Legendre polynomial, $r_{n+1}(y)$, we have the property we need.

Composite Quadrature Rules

Approximating the integrand with a PP leads to the class of Composite Rules. Let $a = x_0 < \cdots x_M = b$ and $S(x)$ be a PP approximation to $f(x)$ (defined on this mesh). We can then use $\int_a^b S(x)dx$ as the approximation to $I(f) = \int_a^b f(x)dx$. Recall that $S(x) \equiv p_{i,n}(x)$ for $x \in [x_{i-1}, x_i]$ $i = 1, \cdots M$. From calculus we have,

$$\int_a^b S(x)dx = \sum_{i=1}^{M} \int_{x_{i-1}}^{x_i} S(x)dx \quad = \sum_{i=1}^{M} \int_{x_{i-1}}^{x_i} p_{i,n}(x)dx,$$

–A sum of basic interpolatory rules.

If we use equally spaced x_i's and low degree interpolation we obtain familiar rules.

Error Estimates for GQ

Let $G_n(f) = \sum_{i=0}^{n} \omega_i f(x_i)$ denote the $(n+1)$ – point Gaussian quadrature rule.

- We have shown,

$$I(f) - G_n(f) = O(b-a)^{2n+3}, \text{ as } (b-a) \to 0.$$

- The rules $G_{n+1}, G_{n+2}, \cdots$, are more accurate (as $(b-a) \to 0$) so we could use,

$$\widehat{EST}_{G_n} \equiv G_{n+k}(f) - G_n(f) = E_{G_n} + O(b-a)^{2(n+k)+3}.$$

- The rules G_{n+k} and G_n have at most one common interpolation point so the computation of this error estimate more than doubles the cost ($2n+k+2$ integrand evaluations).

Error Est for GQ (cont)

- An alternative (to forming an error estimate based on G_{n+k}) is to use the integrand evaluations already available (for the computation of $G_n(f)$) and introduce only the minimum number of extra evaluations required to obtain an effective error estimate.
- This approach leads to a class of quadrature rules called Kronrod quadrature rules, $K_{n+k}(f)$. The error estimate for $G_n(f)$, is then $K_{n+k}(f) - G_n(f)$, where $K_{n+k}(f)$ is more accurate <u>and</u> less expensive to compute than is $G_{n+k}(f)$. Kronrod proposed a particularly effective class of such rules where $k = n + 1$,

$$K_{2n+1}(f) \equiv \sum_{i=0}^{n} a_i f(x_i) + \sum_{j=0}^{n+1} b_j f(y_j),$$

$K_{2n+1}(f) \equiv \sum_{i=0}^{n} a_i f(x_i) + \sum_{j=0}^{n+1} b_j f(y_j)$

- The $x_i's$ are the interpolation points associated with $G_n(f)$, and the y_i's are the extra interpolation points necessary to define an accurate approximation to $I(f)$. Kronrod derived these weights (the a_i's and the b_i's) and the extra interpolation points $(y_0, y_1, \cdots y_n)$ so that the resulting rule is order $3n+3$.
- The resulting error estimate is then,

$$EST_{G_n} \equiv K_{2n+1}(f) - G_n(f),$$

  with an associated cost of $2n+3$ integrand evaluations and an order of accuracy of $O((b-a)^{3n+4})$.
- These Gauss-Kronrod pairs of rules can be the basis for composite quadrature rules and adaptive methods. These methods are widely used and implemented in numerical libraries.

2D Quadrature

- Consider the problem of approximating integrals in two dimensions,

$$I(f) = \int\int_D f(x,y)dxdy,$$

  This problem is more complicated than the one dimensional case since D can take many forms.

- One can develop the analogs of Gaussian rules or interpolatory rules but the weights and nodes will depend on the region D. Such rules can be determined and tabulated for simple regions such as rectangles, triangles and circles.
- An arbitrary region must then be transformed onto one of these simple regions before the rule can be used. Such a transformation will generally be nonlinear and may introduce an approximation error as well.

2D Quadrature (cont)

- An alternative approach is to apply a 'product rule', where one reduces the $2D$-integral to a sequence of two $1D$-integrals:

$$\int_a^b \int_{\alpha(y)}^{\beta(y)} f(x,y)dxdy = \int_a^b g(y)dy,$$

where

$$g(y) \equiv \int_{\alpha(y)}^{\beta(y)} f(x,y)dx.$$

- Note that $g(y)$ is a $1D$-integral with upper and lower bounds depending on y.
- In this case $g(y)$ is approximated, for a fixed value of y, by a standard method (for example, $\approx \sum_{j=0}^{M} \omega_j f(x_j, y)$), and $\int_a^b g(y)dy$ is also approximated by a standard method.

2D Quadrature (cont)

That is,

$$\int_a^b \int_{\alpha(y)}^{\beta(y)} f(x,y)dxdy = \int_a^b g(y)dy \approx \sum_{r=0}^{M'} \hat{\omega}_r g(y_r),$$

$$\approx \sum_{r=0}^{M'} \hat{\omega}_r \left(\sum_{j=0}^{M} \omega_j f(x_j, y_r) \right),$$

$$= \sum_{r=0}^{M'} \sum_{j=0}^{M} (\hat{\omega}_r \omega_j) f(x_j, y_r).$$

Note that error estimates for product rules are not easy to develop since the function $g(y) \approx \sum_{j=0}^{M} \omega_j f(x_j, y)$ will not be a 'smooth' function of y unless M and the x_j's are fixed (which is unlikely since $\alpha(y)$ and $\beta(y)$ are not fixed). In particular this 'inner rule' cannot be adaptive.