Numerical quadrature

Michael S. Floater

May 9, 2016

Abstract

We look at interpolatory quadrature rules and their error, and how to deal with singularities.

In general we would like to approximate the weighted integral

$$I[f] = \int_a^b f(x)w(x)\,dx,$$

of a real function $f : [a,b] \to \mathbb{R}$, with respect to some weight function $w : [a,b] \to \mathbb{R}$, by an n-point quadrature rule

$$I_n[f] = \sum_{i=1}^{n} w_i f(x_i), \tag{1}$$

for certain points $a \le x_1 < x_2 < \cdots < x_n \le b$ and weights $w_i \in \mathbb{R}$. The quadrature rule I_n is *open* if $x_1 > a$ and $x_n < b$, and *closed* if $x_1 = a$ and $x_n = b$. We say that I_n has *degree of precision* d if it is exact for polynomials of degree $\le d$, i.e., that $I_n[p] = I[p]$ for all polynomials p in π_d. It is sufficient to show that $I_n[x^k] = I[x^k]$ for all $k = 0, 1, \ldots, d$.

1 Interpolatory quadrature

Interpolatory quadrature is based on polynomial interpolation. For any choice of points x_i we can find weights w_i for which I_n has degree of precision $\ge n-1$. We do this by integrating the Lagrange interpolant $p \in \pi_{n-1}$ to f at these points, and let

$$I_n[f] := I[p]. \tag{2}$$

Since

$$p(x) = \sum_{i=1}^{n} L_i(x) f(x_i),$$

where

$$L_i(x) = \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j},$$

we obtain the rule

$$I_n[f] = \sum_{i=1}^{n} w_i f(x_i),$$

where $w_i = I[L_i]$. This rule has degree of precision at least $n-1$ because if $f \in \pi_{n-1}$ then $p = f$.

We obtain the error of the quadrature rule from Newton's error formula for polynomial interpolation. Since

$$f(x) - p(x) = (x - x_1) \cdots (x - x_n)[x_1, \ldots, x_n, x]f,$$

the quadrature error is

$$R := I[f] - I_n[f] = \int_a^b (x - x_1) \cdots (x - x_n)[x_1, \ldots, x_n, x]f \, w(x) \, dx.$$

2 Trapezoidal rule

The trapezoidal rule is a 2-point interpolatory quadrature rule, with weight function $w(x) = 1$. Suppose $[a, b] = [0, h]$ and that $f \in C^2[0, h]$, and let $n = 2$, $x_1 = 0$, and $x_2 = h$. Then

$$L_1(x) = \frac{h - x}{h}, \qquad L_2(x) = \frac{x}{h},$$

and

$$w_1 = I[L_1] = h/2, \qquad w_2 = I[L_2] = h/2,$$

and so

$$I_2[f] = \frac{h}{2}(f(0) + f(h)).$$

The error is

$$R = \int_0^h x(x-h)[0,h,x]f\,dx = [0,h,\eta]f\int_0^h x(x-h)\,dx = -f''(\xi)\frac{h^3}{12},$$

for some $\xi \in (0,h)$. Here we have used the mean value theorem for integrals: if $f \in C[a,b]$, g is integrable, and either $g(x) \geq 0$ for all $x \in [a,b]$, or $g(x) \leq 0$ for all $x \in [a,b]$, then there exists some $\eta \in (a,b)$ such that

$$\int_a^b f(x)g(x)\,dx = f(\eta)\int_a^b g(x)\,dx.$$

3 Midpoint rule

The midpoint rule is a 1-point interpolatory quadrature rule, with weight function $w(x) = 1$. Suppose $[a,b] = [-h/2, h/2]$ and that $f \in C^2[-h/2, h/2]$, and let $n = 1$ and $x_1 = 0$. Then

$$L_1(x) = 1, \qquad w_1 = I[L_1] = h,$$

and so

$$I_1[f] = hf(0).$$

The error is

$$R = \int_{-h/2}^{h/2} x[0,x]f\,dx.$$

Notice that R is zero both for constant and linear f, due to the fact that

$$\int_{-h/2}^{h/2} x\,dx = 0. \tag{3}$$

Thus the midpoint rule has degree of precision 1, the same as the trapezoidal rule. We can also use (3) to obtain an error formula in terms of the second derivative of f. We have

$$\begin{aligned} R &= \int_{-h/2}^{h/2} x([0,x]f - [0,0]f)\,dx \\ &= \int_{-h/2}^{h/2} x^2[0,0,x]f\,dx = [0,0,\eta]f\int_{-h/2}^{h/2} x^2\,dx = f''(\xi)\frac{h^3}{24}. \end{aligned} \tag{4}$$

Thus the error of the midpoint rule is half that of the trapezoidal rule, even though it only uses one point.

An alternative way of deriving the midpoint rule is to use Hermite interpolation, and interpolate f by the linear polynomial

$$q(x) = f(0) + xf'(0),$$

and set

$$I_1[f] := I[q].$$

The integral $I[q]$ does not depend on $f'(0)$ because of (3), and we obtain

$$I_1[f] = hf(0),$$

as before. The quadrature error can now be derived from the error formula for Hermite interpolation:

$$R = I[f] - I[q] = \int_{-h/2}^{h/2} (x-0)^2 [0,0,x]f \, dx,$$

which gives (4) more directly.

4 Simpson's rule

Simpson's rule is a 3-point interpolatory quadrature rule, with weight function $w(x) = 1$. Suppose $[a,b] = [-h,h]$ and that $f \in C^4[-h,h]$, and let $n = 3$ and $x_1 = -h$, $x_2 = 0$, $x_3 = h$. Then

$$L_1(x) = \frac{x(x-h)}{2h^2}, \qquad L_2(x) = \frac{h^2 - x^2}{h^2}, \qquad L_3(x) = \frac{x(x+h)}{2h^2},$$

and

$$w_1 = h/3, \qquad w_2 = 4h/3, \qquad w_3 = h/3,$$

and so

$$I_3[f] = \frac{h}{3}(f(-h) + 4f(0) + f(h)).$$

The error is

$$R = \int_{-h}^{h} x(x^2 - h^2)[-h,0,h,x]f \, dx.$$

Since

$$\int_{-h}^{h} x\,dx = \int_{-h}^{h} x^3\,dx = 0, \tag{5}$$

it follows that I_3 has degree of precision 3: it is exact for cubic polynomials. Furthermore, by (5),

$$\begin{aligned} R &= \int_{-h}^{h} x(x^2 - h^2)([-h,0,h,x]f - [-h,0,h,0]f)\,dx \\ &= \int_{-h}^{h} x^2(x^2 - h^2)[-h,0,0,h,x]f\,dx = -f^{(4)}(\xi)\frac{h^5}{90}. \end{aligned} \tag{6}$$

Similar to the midpoint rule, Simpson's rule and its error can also be derived by interpolating f with the cubic polynomial q such that

$$q(-h) = f(-h), \quad q(0) = f(0), \quad q'(0) = f'(0), \quad q(h) = f(h),$$

and letting $I_3[f] := I[q]$.

5 Composite rules

We can derive composite quadrature rules by dividing the interval of integration and applying a polynomial-based rule, as above, to each subinterval.

For example, for the composite trapezoidal rule, let $x_i = a + ih$, $i = 0, 1, \ldots, n$, where $h = (b-a)/n$, and suppose $f \in C^2[a,b]$, and let $f_i = f(x_i)$. Then from the trapezoidal rule applied to each sub-interval $[x_i, x_{i+1}]$,

$$I[f] = \sum_{i=0}^{n-1} \frac{h}{2}(f_i + f_{i+1}) - \sum_{i=0}^{n-1} \frac{h^3}{12} f''(\xi_i),$$

for some $\xi_i \in (x_i, x_{i+1})$, $i = 0, \ldots, n-1$. Thus,

$$I[f] = T(h) + R_T,$$

where $T(h)$ is the composite trapeoidal rule,

$$T(h) = \frac{h}{2}(f_0 + f_n) + h \sum_{i=1}^{n-1} f_i,$$

and, by the mean value theorem,

$$R_T = -\frac{h^3}{12}\sum_{i=0}^{n-1} f''(\xi_i) = -\frac{h^3}{12} n f''(\eta) = -(b-a)\frac{h^2}{12} f''(\eta),$$

for some $\eta \in (a,b)$.

Similarly, applying the midpoint rule to each interval (x_i, x_{i+1}) gives

$$I[f] = M(h) + R_M,$$

where $M(h)$ is the composite midpoint rule,

$$M(h) = h\sum_{i=0}^{n-1} f_{i+1/2},$$

and $f_{i+1/2} := f(x_{i+1/2})$, $x_{i+1/2} := a + (i+1/2)h$, and

$$R_M = (b-a)\frac{h^2}{24} f''(\eta).$$

For the composite Simpson's rule, suppose $n = 2m$. Then

$$I[f] = \sum_{i=0}^{m-1}\int_{x_{2i}}^{x_{2i+1}} f(x)\,dx = S(h) + R_S,$$

where

$$S(h) = \sum_{i=0}^{m-1}\frac{h}{3}(f_{2i} + 4f_{2i+1} + f_{2i+2}) = \frac{h}{3}(f_0 + 4S_1 + 2S_2 + f_n),$$

and

$$S_1 = f_1 + f_3 + \cdots + f_{n-1}, \qquad S_2 = f_2 + f_4 + \cdots + f_{n-2},$$

and,

$$R_S = -\frac{h^5}{90}\sum_{i=0}^{m-1} f^{(4)}(\xi_i) = -\frac{h^5}{90} m f^{(4)}(\eta) = -(b-a)\frac{h^4}{180} f''(\eta).$$

Notice that

$$T(2h) = hf_0 + 2hS_2 + hf_n, \qquad M(2h) = 2hS_1,$$

and therefore

$$S(h) = \frac{T(2h) + 2M(2h)}{3}.$$

6 Singularities

If the integrand has a singularity, the usual quadrature rules will typically be inaccurate, and sometimes may not even be valid. Singularities can sometimes be treated by a transformation which improves the integrand. For example, the integral

$$I = \int_0^1 \frac{1}{\sqrt{x}} e^x \, dx$$

can be transformed by the substitution $x = t^2$, so that

$$I = 2 \int_0^1 e^{t^2} \, dt.$$

Alternatively, the singularity can be weakened by integration by parts:

$$I = \int_0^1 x^{-1/2} e^x \, dx = \left[2x^{1/2} e^x\right]_0^1 - 2 \int_0^1 x^{1/2} e^x \, dx = 2 - 2 \int_0^1 x^{1/2} e^x \, dx,$$

and further integration by parts would weaken the singularity further.

Another approach is to use a weight function. For example, to integrate

$$I = \int_0^{2h} x^{-1/2} f(x) \, dx,$$

we could let $w(x) = x^{-1/2}$, and then

$$I[f] = \int_0^{2h} w(x) f(x) \, dx.$$

Let us consider the 'weighted' version of Simpson's rule. With $n = 3$ and $x_1 = 0$, $x_2 = h$, $x_3 = 2h$,

$$L_1(x) = \frac{(x-h)(x-2h)}{2h^2}, \qquad L_2(x) = -\frac{x(x-2h)}{h^2}, \qquad L_2(x) = \frac{x(x-h)}{2h^2}.$$

Then

$$w_k = \int_0^{2h} x^{-1/2} L_k(x) \, dx, \qquad k = 1, 2, 3,$$

and we find

$$(w_1, w_2, w_3) = \frac{2^{1/2} h^{1/2}}{15} (12, 16, 2),$$

and so

$$I_3[f] = \frac{2^{1/2}h^{1/2}}{15}(12f(0) + 16f(h) + 2f(2h)),$$

which has degree of precision 2. The error is

$$R = I[f] - I_3[f] = \int_0^{2h} x^{1/2}(x-h)(x-2h)[0,h,2h,x]f\,dx,$$

which is $O(h^{7/2})$ as $h \to 0$ if $f \in C^3[0,1]$.