Quadrature Rules from an Advanced Perspective

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1 Introduction

The purpose of this note is to examine numerical quadrature rules and their errors. The perspective here is that a numerical quadrature rule is integration with respect to a purely atomic measure. For the purpose of this discussion all functions and measures will be defined on the unit interval. Recall that typically an interval of integration will be subdivided into contiguous short intervals and the result of quadrature applied over each of these short intervals will be combined to provide an estimate of the original integral. The unit interval in this discussion may be viewed as a prototype for one of these short intervals.

Extensions of this discussion to the interval $[a,b]$ can be made by using a linear change of variables $\int_a^b f(x)\,dx = (b-a)\int_0^1 f(a+(b-a)x)\,dx$. Thus the values and derivatives of the function f occurring below would be replaced by the values and derivatives of the function $(b-a)f(a+(b-a)x)$.

2 The Basic Method

One method of devising a quadrature rule is to require that the rule give exact results for polynomials of a particular degree or less. The rectangle rule satisfies this requirement for constants, that is, polynomials of degree 0. Clearly a measure integrating constants exactly is only required to give the unit interval unit mass.

The first step in the analysis is to obtain a formula which will be useful in determing the error when using a particular quadrature formula. Suppose f is a smooth function and ν is a finite measure. Using the Fundamental Theorem of Calculus and Fubini's Theorem gives

$$\begin{aligned}\int_0^1 f(x)\,d\nu(x) &= \int_0^1 \left(f(0)+\int_0^x f'(t)\,dt\right) d\nu(x)\\ &= f(0)\,\nu([0,1])+\int_0^1\int_0^x f'(t)\,dt\,d\nu(x)\\ &= f(0)\,\nu([0,1])+\int_0^1\int_t^1 f'(t)\,d\nu(x)\,dt\\ &= f(0)\,\nu([0,1])+\int_0^1 f'(t)\,\nu([t,1])\,dt.\end{aligned}$$

The error of a particular quadrature rule will be obtained by considering what this formula yields when ν is Lebesgue measure as compared with the atomic measure corresponding to the quadrature rule.

3 The Rectangle Rules

As a first use, consider the rectangle rule based on right hand endpoints. The atomic measure corresponding to this rule is $\rho = \delta_1$, the unit point mass at 1. Using the formula above and alternately substituting Lebesgue measure and ρ for ν yields

$$\begin{aligned}\int_0^1 f(x)\,dx - f(1)(1-0) &= \int_0^1 f(x)\,dx - \int_0^1 f(x)\,d\rho(x)\\ &= \int_0^1 f'(t)\,((1-t)-\rho([t,1]))\,dt\\ &= \int_0^1 f'(t)(-t)\,dt\end{aligned}$$

since $\rho([t,1]) = 1$. Simple estimation shows that this error does not exceed $\sup|f'|\int_0^1 |-t|\,dt = \sup|f'|/2$.

The rectangle rule with left endpoints corresponds to the measure $\lambda = \delta_0$, and the same argument gives

$$\int_0^1 f(x)\,dx - f(0)(1-0) = \int_0^1 f(x)\,dx - \int_0^1 f(x)\,d\lambda(x)$$

$$= \int_0^1 f'(t)\,((1-t)-\lambda([t,1]))\,dt$$
$$= \int_0^1 f'(t)(1-t)\,dt$$

since $\lambda([t,1]) = 0$. Simple estimation shows that this error does not exceed $\sup|f'| \int_0^1 |1-t|\,dt = \sup|f'|/2$.

4 The Midpoint and Trapezoid Rules

Other simple quadrature rules, such as the midpoint and trapezoid rule, produce exact results when integrating first degree polynomials, not just constants like the two rectangle rules. This suggests that the basic formula should be expanded by using two terms of the Maclaurin expansion of the integrand instead of one. The form of the Maclaurin expansion is that obtained by iterating the Fundamental Theorem, as

$$\begin{aligned} f(x) &= f(0) + \int_0^x f'(t)\,dt \\ &= f(0) + \int_0^x \left(f'(0) + \int_0^t f''(s)\,ds \right) dt \\ &= f(0) + f'(0)x + \int_0^x \int_0^t f''(s)\,ds\,dt. \end{aligned}$$

Proceeding now as in the derivation of the basic formula gives

$$\begin{aligned} \int_0^1 f(x)\,d\nu(x) = {} & f(0)\,\nu([0,1]) \\ & + f'(0) \int_0^1 x\,d\nu(x) \\ & + \int_0^1 f''(s) \left(\int_s^1 \int_t^1 d\nu(x)\,dt \right) ds. \end{aligned}$$

Comparing Lebesgue measure with the midpoint rule's measure $\mu = \delta_{1/2}$ gives the error as not exceeding

$$\sup|f''| \int_0^1 \left| \int_s^1 \int_t^1 dx\,dt - \int_s^1 \int_t^1 d\mu(x)\,dt \right| ds.$$

Since $\mu([t,1])$ is either 0 or 1 according as $t > 1/2$ or $t \leq 1/2$, the integral can be readily computed to be $1/24$.

For the trapezoid rule's measure $\tau = \frac{1}{2}\delta_0 + \frac{1}{2}\delta_1$, the error does not exceed

$$\sup|f''| \int_0^1 \left| \int_s^1 1 - t - \tau([t,1])\, dt \right| ds.$$

Since $\tau([t,1]) = 1/2$ the integral is computed as $1/12$. The midpoint rule is generally the better of these two rules.

5 Simpson's Rule and Two Point Gaussian Quadrature

Simpson's rule integrates polynomials of third degree exactly and corresponds to the measure $\sigma = \frac{1}{6}\delta_0 + \frac{4}{6}\delta_{1/2} + \frac{1}{6}\delta_1$. Using a fourth degree Maclaurin expansion as above shows that the error using Simpson's rule does not exceed

$$\sup|f''''| \int_0^1 \left| \int_q^1 \int_r^1 \int_s^1 \int_t^1 dx\, dt\, ds\, dr - \int_q^1 \int_r^1 \int_s^1 \int_t^1 d\sigma(x)\, dt\, ds\, dr \right| dq$$

While rather complicated, the multiple integral can be evaluated as $1/2880$.

Finally, the two point Gaussian quadrature, corresponding to the measure $\gamma = \frac{1}{2}\delta_{(3-\sqrt{3})/6} + \frac{1}{2}\delta_{(3+\sqrt{3})/6}$, also integrates third degree polynomials exactly. The same argument as in the case of Simpson's rule shows that the error does not exceed $\sup|f''''|/4320$.

6 Conclusion

The perspective provided above yields a simple, mechanically expandable form for the error of any numerical quadrature method that can be expressed as an integral with respect to an atomic measure. Explicit computation of the resulting error bound may be done by hand in simple cases, or by using software capable of symbolic computation.