Numerical Integration

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1 Introduction to Quadrature

Our goal is to approximate the definite integral of a function $f(x)$ over an interval $[a,b]$ by evaluating $f(x)$ at a finite number of sample points.

Definition 1 *Suppose that $a = x_0 < x_1 < \ldots < x_n = b$ and that $\{w_k\}_{k=0}^{n}$ is a set of real numbers. A formula of the form*

$$Q[f] = \sum_{k=0}^{n} w_k f(x_k)$$

is called a quadrature formula. The points $\{x_k\}_{k=0}^{n}$ are called the quadrature nodes and the numbers $\{w_k\}_{k=0}^{n}$ are called the weights.

What we have in mind is that

$$\int_a^b f(x)\,dx \approx \sum_{k=0}^{n} w_k f(x_k).$$

The error

$$E[f] = \int_a^b f(x)\,dx - Q[f]$$

is called the truncation error.

Definition 2 *If a quadrature formula is such that*

$$\int_a^b P_i(x)\,dx = Q[P_i]$$

for all polynomials $P_i(x)$ of degree $i \leq n$ but

$$\int_a^b P_{n+1}(x)\,dx \neq Q[P_{n+1}]$$

for some polynomial $P_{n+1}(x)$ of degree $n+1 \neq 0$ then we say that the <u>degree of precision</u> of the quadrature formula is n.

One way to obtain quadrature formulas is to interpolate f at the nodes $\{x_k\}_{k=0}^n$ and integrate the interpolating polynomial. For example, if we use Lagrange interpolation, then we have

$$f(x) \approx \sum_{k=0}^{n} f(x_k) L_{k,n}(x)$$

and hence,

$$\begin{aligned}\int_a^b f(x)\,dx &\approx \int_a^b \sum_{k=0}^{n} f(x_k) L_{k,n}(x)\,dx \\ &= \sum_{k=0}^{n} f(x_k) \int_a^b L_{k,n}(x)\,dx \\ &= \sum_{k=0}^{n} w_k f(x_k).\end{aligned}$$

So, the weights turn out to be the integrals of the basic Lagrange polynomials. Observe that if $f(x)$ is already a polynomial of degree $i \leq n$, then

$$P_i(x) = \sum_{k=0}^{n} P_i(x_k) L_{k,n}(x)$$

and hence,

$$\int_a^b P_i(x)\,dx = \sum_{k=0}^{n} w_k P_i(x_k).$$

Therefore, interpolating with a polynomial of degree n produces quadrature formulas with degree of precision at least n.

The truncation error can also be anticipated from the error for the Lagrange interpolation. Since

$$\begin{aligned}f(x) &= \sum_{k=0}^{n} f(x_k) L_{k,n}(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{k=0}^{n} (x - x_k), \\ \int_a^b f(x)\,dx &= Q[f] + \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{k=0}^{n} (x - x_k)\,dx,\end{aligned}$$

using a mean value theorem for integrals, we get

$$\begin{aligned}\int_a^b f(x)\,dx &= Q[f] + \frac{f^{(n+1)}(\eta)}{(n+1)!} \int_a^b \prod_{k=0}^{n} (x - x_k)\,dx \\ &= Q[f] + C f^{(n+1)}(\eta),\end{aligned}$$

where

$$C = \frac{1}{(n+1)!} \int_a^b \prod_{k=0}^{n} (x - x_k)\,dx$$

and $\eta \in [a, b]$. Thus

$$E[f] = Cf^{(n+1)}(\eta).$$

Quadrature rules obtained this way are called *Newton-Cotes* formulas. When the nodes $x_0 = a$ and $x_n = b$ are used, it is called a *closed Newton-Cotes* formula. Supposing that the nodes are equally spaced and that $h = x_1 - x_0$, the first four closed Newton-Cotes formulas are

$$\begin{array}{ll}
\int_{x_0}^{x_1} f(x)\,dx \approx \frac{h}{2}(f_0 + f_1) & \text{(trapezoidal rule)}, \\
\int_{x_0}^{x_1} f(x)\,dx \approx \frac{h}{3}(f_0 + 4f_1 + f_2) & \text{(Simpson's rule)}, \\
\int_{x_0}^{x_1} f(x)\,dx \approx \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) & \text{(Simpson's } \tfrac{3}{8}\text{rule)}, \\
\int_{x_0}^{x_1} f(x)\,dx \approx \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) & \text{(Boole's rule)}.
\end{array}$$

and the errors take the form

$$-\frac{h^3}{12}f^{(2)}(\eta), -\frac{h^5}{90}f^{(4)}(\eta), -\frac{3h^5}{80}f^{(4)}(\eta), -\frac{8h^7}{945}f^{(6)}(\eta),$$

respectively. Note that the degrees of precision are $n = 1, n = 3, n = 3, n = 4$, respectively. Here we used the now standard notation

$$f_k = f(x_k).$$

The computation of the weights involves the "tedious" integration of the basic Lagrange polynomials. Symbolic manipulators may be of help here. To illustrate, we show the Maple Commands taken to produce the weights for Simpson's rule.

$$\int_{x_0}^{x_2} L_{0,2}(x)\,dx = \int_{x_0}^{x_2} \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}dx = -\frac{1}{6}\frac{(x_0 - x_2)(2x_0 - 3x_1 + x_2)}{(x_0 - x_1)} = \frac{h}{3}$$

and the command used to produce this result is

```
> factor(int((x-x1)*(x-x2)/(x0-x1)/(x0-x2),x=x0..x2));
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$$\int_{x_0}^{x_2} L_{1,2}(x)\,dx = \int_{x_0}^{x_2} \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}dx = \frac{1}{6}\frac{(x_0 - x_2)^3}{(x_0 - x_1)(x_2 - x_1)} = \frac{4h}{3}$$

and the Maple command used to produce this result is

```
> factor(int((x-x0)*(x-x2)/(x1-x0)/(x1-x2),x=x0..x2));
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$$\int_{x_0}^{x_2} L_{2,2}(x)\,dx = \int_{x_0}^{x_2} \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}dx = -\frac{1}{6}\frac{(x_0 - x_2)(x_0 - 3x_1 + 2x_2)}{(x_2 - x_1)} = \frac{h}{3}.$$

Therefore,

$$\begin{aligned}
\int_{x_0}^{x_2} f(x)\,dx &\approx \sum_{k=0}^{2} f(x_k) \int_a^b L_{k,2}(x)\,dx \\
&= \frac{h}{3}(f_0 + 4f_1 + f_2).
\end{aligned}$$

Example For the function $f(x) = 1 + e^{-x}\sin(4x)$, the exact value of

$$\int_0^1 f(x)\,dx = \int_0^1 (1 + e^{-x}\sin(4x))dx = 1.308250605.$$

1. Using the Trapezoidal Rule,

$$\int_0^1 f(x)\,dx \approx \frac{1}{2}\left[(1) + \left(1 + e^{-1}\sin 4\right)\right] = .8607939604.$$

2. Using Simpson's Rule,

$$\begin{aligned}\int_0^1 f(x)\,dx &\approx \frac{1}{9}\left[1 + 4\left(1 + e^{-1l2}\sin 2\right) + \left(1 + e^{-1}\sin 4\right)\right] \\ &= 1.321275832.\end{aligned}$$

3. Using Simpson's $\frac{3}{8}$ Rule,

$$\int_0^1 f(x)\,dx \approx \frac{3}{8}(1/3)\left(f(0) + 3f(1/3) + 3f(2/3) + f(1)\right) = 1.314396815.$$

4. Using Boole's Rule,

$$\begin{aligned}\int_0^1 f(x)\,dx &\approx \frac{2}{45}(1/4)\left(7f(0) + 32f(1/4) + 12f(2/2) + 32f(3/4) + 7f(1)\right) \\ &= 1.308591922.\end{aligned}$$

As expected, the approximation from Boole's rule is the best.

2 Composite Trapezoidal and Simpson's Rules

The error formula for the quadrature rules we saw in the previous sections are dependent on the width h of the subintervals entering into the quadrature rule. The smaller h is the smaller the error is and, consequently the more accurate the approximation is. Thus to more accurate approximations of the integral $\int_a^b f(x)\,dx$ we divide this interval into integrals over smaller integrals, approximate each integral and then add the results. In this section we will discuss the repeated use of the trapezoidal rule (composite trapezoindal rule) and Simpson's rule (composite Simpson's rule) and estimate the resulting errors.

2.1 The composite trapezoidal rule

For the trapezoidal rule we divide the interval $[a, b]$ into M equal subintervals using M $+1$ equally spaced nodes $a = x_0 < x_1 < \ldots < x_M = b$. Then the composite trapezoidal rule is pbtained as follows:

$$\begin{aligned}
\int_a^b f(x)\,dx &= \int_{x_0}^{x_M} f(x)\,dx = \sum_{k=1}^{M} \int_{x_{k-1}}^{x_k} f(x)\,dx \\
&\approx \sum_{k=1}^{M} \frac{h}{2}(f_k + f_{k-1}) \qquad (1)\\
&= \frac{h}{2}(f_0 + 2f_1 + 2f_2 + \ldots + 2f_{M-1} + f_M) \qquad (2)\\
&= \frac{h}{2}(f_0 + f_M) + h \sum_{k=1}^{M-1} f_k. \qquad (3)
\end{aligned}$$

All three forms (1)-(3) are interchangeably used.

Example For the function $f(x) = 2 + \sin(2\sqrt{x})$ over the interval $[1, 6]$ with 11 nodes, the width of each subinterval $h = \frac{6-1}{10} = 0.5$. Thus

$$\begin{aligned}
\int_1^6 f(x)\,dx &\approx 0.25(f_0 + f_{10}) + 0.5 \sum_{k=1}^{10} f_k \\
&= 0.25(2.909297427 + 1.01735756) \\
&\quad +.5(2.638157635 + 2.308071742 + 1.979316468) \\
&\quad +.5(1.683052837 + 1.435304101 + 1.243197505) \\
&\quad +.5(1.108317746 + 1.028722201 + 1.000241401) \\
&= 8.193854565.
\end{aligned}$$

The exact value of the integral is 8.183479208.

To obtain the error formula, we recall that the error is obtained over the k^{th} subinterval by integrating the truncation error of the Lagrange interpolation. This gives

$$\begin{aligned}
E_k[f] &= \int_{x_{k-1}}^{x_k} \frac{(x - x_{k-1})(x - x_k)}{2} f^{(2)}(\xi(x))\,dx \\
&= \frac{1}{2} \int_{x_{k-1}}^{x_k} (x - x_{k-1})(x - x_k) f^{(2)}(\xi(x))\,dx.
\end{aligned}$$

Observe that the quantity $(x - x_{k-1})(x - x_k)$ does not change signs on the interval $[x_{k-1}, x_k]$. Then, by the second mean value theorem for integrals, there is a $c_k \in [x_{k-1}, x_k]$ such that

$$\begin{aligned}
E_k[f] &= \frac{f^{(2)}(c_k)}{2} \int_{x_{k-1}}^{x_k} (x - x_{k-1})(x - x_k)\,dx \\
&= -\frac{h^3}{12} f^{(2)}(c_k).
\end{aligned}$$

Thus, the overall truncation error is

$$\begin{aligned} E[f] &= \sum_{k=1}^{M} E_k[f] = -\frac{h^3}{12}\sum_{k=1}^{M} f^{(2)}(c_k) \\ &= -\frac{h^3}{12} M \sum_{k=1}^{M} \frac{1}{M} f^{(2)}(c_k). \end{aligned}$$

Since $\sum_{k=1}^{M} \frac{1}{M} f^{(2)}(c_k)$ is an average value of the second derivatives involved, it lies between the minimum and maximum of these derivatives. Therefore, by the intermediate value theorem applied to $f^{(2)}(x)$, we get that there exists a value $c \in [a, b]$ such that

$$\sum_{k=1}^{M} \frac{1}{M} f^{(2)}(c_k) = f^{(2)}(c).$$

Therefore,

$$\begin{aligned} E[f] &= -\frac{h^3}{12} M f^{(2)}(c) \\ &= -\frac{h^3}{12}\frac{(b-a)}{h} f^{(2)}(c) \\ &= -\frac{(b-a)}{12} h^2 f^{(2)}(c). \end{aligned}$$

2.2 The composite Simpson's rule

Since Simpson's rule requires integration over two subintervals at a time, the interval $[a, b]$ should be divided into $2M$ subintervals by $2M+1$ nodes $a = x_0 < x_1 < \ldots < x_{2M} = b$.. Proceeding in a similar way to the composite trapezoidal rule we obtain

$$\begin{aligned} \int_a^b f(x)\,dx &= \int_{x_0}^{x_{2M}} f(x)\,dx \\ &= \sum_{k=1}^{M} \int_{x_{2k-2}}^{x_{2k}} f(x)\,dx \\ &\approx \frac{h}{3}\sum_{k=1}^{M} f_{2k-2} + 4f_{2k-1} + f_{2k} \\ &= \frac{h}{3}\sum_{k=1}^{M} f_{2k-2} + f_{2k} + \frac{4h}{3}\sum_{k=1}^{M} f_{2k-1} \\ &= \frac{h}{3}(f_0 + f_{2M}) + \frac{2h}{3}\sum_{k=1}^{M-1} f_{2k} + \frac{4h}{3}\sum_{k=1}^{M} f_{2k-1} \end{aligned}$$

It can be shown that the truncation error for the composite Simpson's rule is

$$E[f] = -\frac{(b-a)}{180} f^{(4)}(c)\, h^4 = O\left(h^4\right). \tag{4}$$

Example If the composite Simpson's rule is applied to the function $f = 1/x$ over the interval $[2, 7]$, find the number of subintervals M and the width h so that the approximation error does not exceed $5 * 10^{-9}$.

Applying the error formula (4) we compute

$$f^{(4)}(x) = \frac{24}{x^5}.$$

Hence,

$$\left|f^{(4)}(x)\right| \leq \frac{24}{2^5} = \frac{3}{4}.$$

Thus we require that

$$\frac{(7-2)}{180} \times \frac{3}{4} \times h^4 \leq 5 * 10^{-9}.$$

This yeilds

$$h \approx .0007$$

and

$$M = \frac{b-a}{h} = \frac{5000}{7} = 714.29$$

Since M must be an even integer, we choose

$$M = 716$$

and

$$h = \frac{5}{716} = 6.9832 \times 10^{-3}.$$