Numerical Integration

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May 21, 2013

Elements of Numerical Integration

The basic method involved in approximating the integration

$$\int_a^b f(x)\,dx, \tag{1}$$

is called numerical quadrature and uses a sum of the type

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i). \tag{2}$$

The method of quadrature in this section is based on the polynomial interpolation. We first select a set of distinct nodes $\{x_0, x_1, \ldots, x_n\}$ from the interval $[a, b]$. Then the Lagrange polynomial

$$P_n(x) = \sum_{i=0}^{n} f(x_i) L_i(x) = \sum_{i=0}^{n} f(x_i) \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

is used to approximate $f(x)$.

Then

$$f(x) = P_n(x) + E_n(x) = \sum_{i=0}^{n} f(x_i) L_i(x) + \frac{f^{(n+1)}(\zeta_x)}{(n+1)!} \prod_{i=0}^{n} (x - x_i),$$

where $\zeta_x \in [a, b]$ and depends on x, and

$$\begin{aligned} \int_a^b f(x)\,dx &= \int_a^b P_n(x)\,dx + \int_a^b E_n(x)\,dx \\ &= \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)\,dx + \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\zeta_x) \prod_{i=0}^{n} (x - x_i \end{aligned}$$

The quadrature formula is, therefore,

$$\int_a^b f(x)\,dx \approx \int_a^b P_n(x)\,dx = \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)\,dx \equiv \sum_{i=0}^{n} c_i f(x_i), \quad (4)$$

where

$$c_i = \int_a^b L_i(x)\,dx = \int_a^b \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}\,dx. \quad (5)$$

Let us consider formulas produced by using first and second Lagrange polynomials with equally spaced nodes. This gives the Trapezoidal rule and Simpson's rule, respectively.

Trapezoidal rule: Let $x_0 = a, x_1 = b, h = b - a$ and use the linear Lagrange polynomial:

$$P_1(x) = \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1).$$

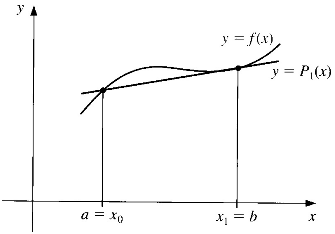
Then

$$\begin{aligned} \int_a^b f(x)dx &= \int_{x_0}^{x_1} \left[\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right] dx \\ &\quad + \frac{1}{2} \int_{x_0}^{x_1} f''(\zeta(x))(x - x_0)(x - x_1)dx. \end{aligned} \tag{6}$$

Consequently, Eq. (6) implies that

$$\begin{aligned}\int_a^b f(x)dx &= \left[\frac{(x-x_1)^2}{2(x_0-x_1)}f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)}f(x_1)\right]_{x_0}^{x_1} - \frac{h^3}{12}f''(\zeta) \\ &= \frac{x_1-x_0}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12}f''(\zeta) \\ &= \frac{h}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12}f''(\zeta),\end{aligned}$$

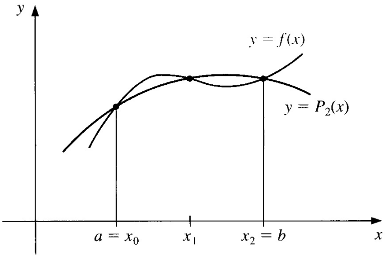
which is called the Trapezoidal rule.



If we choose $x_0 = a$, $x_1 = \frac{1}{2}(a+b)$, $x_2 = b$, $h = (b-a)/2$, and the second order Lagrange polynomial

$$\begin{aligned} P_2(x) &= f(x_0)\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \\ &\quad + f(x_2)\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \end{aligned}$$

to interpolate $f(x)$, then



$$
\begin{aligned}
\int_a^b f(x)dx &= \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \right. \\
&\quad \left. + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx \\
&\quad + \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\zeta(x))dx.
\end{aligned}
$$

Since, letting $x = x_0 + th$,

$$
\begin{aligned}
\int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} dx &= h \int_0^2 \frac{t-1}{0-1} \cdot \frac{t-2}{0-2}\, dt \\
&= \frac{h}{2} \int_0^2 (t^2 - 3t + 2)\, dt = \frac{h}{3}, \\
\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} dx &= h \int_0^2 \frac{t-0}{1-0} \cdot \frac{t-2}{1-2}\, dt \\
&= -h \int_0^2 (t^2 - 2t)\, dt = \frac{4h}{3},
\end{aligned}
$$

$$
\begin{aligned}
\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} dx &= h \int_0^2 \frac{t-0}{2-0} \cdot \frac{t-1}{2-1}\, dt \\
&= \frac{h}{2} \int_0^2 (t^2 - t)\, dt = \frac{h}{3},
\end{aligned}
$$

it implies that

$$
\begin{aligned}
\int_a^b f(x)dx &= h\left[\frac{1}{3} f(x_0) + \frac{4}{3} f(x_1) + \frac{1}{3} f(x_2)\right] \\
&\quad + \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\zeta(x))dx,
\end{aligned}
$$

which is called the Simpson's rule and provides only an $O(h^4)$ error term involving $f^{(3)}$.

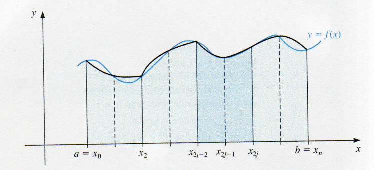
We choose an even integer n and partition the interval $[a, b]$ into n subintervals by nodes $a = x_0 < x_1 < \cdots < x_n = b$, and apply Simpson's rule on each consecutive pair of subintervals. With

$$h = \frac{b-a}{n} \quad \text{and} \quad x_j = a + jh, \quad j = 0, 1, \ldots, n,$$

we have on each interval $[x_{2j-2}, x_{2j}]$,

$$\int_{x_{2j-2}}^{x_{2j}} f(x)\,dx = \frac{h}{3}\left[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})\right] - \frac{h^5}{90} f^{(4)}(\xi_j),$$

for some $\xi_j \in (x_{2j-2}, x_{2j})$, provided that $f \in C^4[a, b]$.



The composite rule is obtained by summing up over the entire interval, that is,

$$
\begin{aligned}
\int_a^b f(x)\,dx &= \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)\,dx \\
&= \sum_{j=1}^{n/2} \left[\frac{h}{3} \left(f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j}) \right) - \frac{h^5}{90} f^{(4)}(\xi_j) \right] \\
&= \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2) \\
&\quad + f(x_2) + 4f(x_3) + f(x_4) \\
&\quad + f(x_4) + 4f(x_5) + f(x_6) \\
&\quad \vdots \\
&\quad + f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)] - \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j)
\end{aligned}
$$

Hence

$$\begin{aligned}\int_a^b f(x)\,dx &= \frac{h}{3}\left[f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+2f(x_4)+4f(x_5)\right. \\ &\quad \left.+\cdots+2f(x_{n-2})+4f(x_{n-1})+f(x_n)\right] - \frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j) \\ &= \frac{h}{3}\left[f(x_0)+4\sum_{j=1}^{n/2} f(x_{2j-1})+2\sum_{j=1}^{(n/2)-1} f(x_{2j})+f(x_n)\right] \\ &\quad -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j).\end{aligned}$$

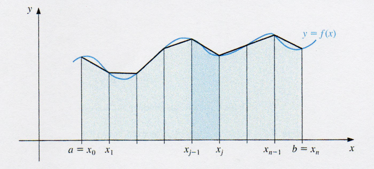
Composite Simpson's Rule

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + f(b)\right] - \frac{b-a}{180} f^{(4)}(\mu) h^4,$$

where n is an even integer, $h = (b-a)/n$, $x_j = a + jh$, for $j = 0, 1, \ldots, n$, and some $\mu \in (a, b)$.

To derive the composite Trapezoidal rule, we partition $[a, b]$ by n equally spaced nodes $a = x_0 < x_1 < \cdots < x_n = b$, where n can be either odd or even. Apply the trapezoidal rule on $[x_{j-1}, x_j]$ and sum them up to obtain

$$\begin{aligned}
\int_a^b f(x)\,dx &= \sum_{j=1}^{n} \int_{x_{j-1}}^{x_j} f(x)\,dx \\
&= \sum_{j=1}^{n} \left\{ \frac{h}{2} \left[f(x_{j-1}) + f(x_j) \right] - \frac{h^3}{12} f''(\xi_j) \right\} \\
&= \frac{h}{2} \{ [f(x_0) + f(x_1)] + [f(x_1) + f(x_2)] + \cdots \\
&\quad + [f(x_{n-1}) + f(x_n)] \} - \frac{h^3}{12} \sum_{j=1}^{n} f''(\xi_j)
\end{aligned}$$



Hence,

$$\begin{aligned}\int_a^b f(x)\,dx &= \frac{h}{2}\left[f(x_0)+2f(x_1)+2f(x_2)+\cdots+2f(x_{n-1})+f(x_n)\right] \\ &\quad -\frac{h^3}{12}\sum_{j=1}^{n} f''(\xi_j) \\ &= \frac{h}{2}\left[f(a)+2\sum_{j=1}^{n-1} f(x_j)+f(b)\right]-\frac{h^3}{12}\sum_{j=1}^{n} f''(\xi_j) \\ &= \frac{h}{2}\left[f(a)+2\sum_{j=1}^{n-1} f(x_j)+f(b)\right]-\frac{b-a}{12}f''(\mu)h^2,\end{aligned}$$

where each $\xi_j \in (x_{j-1}, x_j)$ and $\mu \in (a, b)$.

Composite Trapezoidal Rule

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12} f''(\mu)h^2, \qquad (7)$$

where n is an integer, $h = (b-a)/n$, $x_j = a + jh$, for $j = 0, 1, \ldots, n$, and some $\mu \in (a, b)$.

Program

Use the composite Trapezoidal or Simpson's rule to approximate the integral

$$\text{(a)}. \int_e^{e+2} \frac{1}{x \ln x} dx, \qquad \text{(b)}. \int_{0.75}^{1.75} \left(\sin^2 x - 2x \sin x + 1\right) dx.$$

Requirement:

- Use *function* command to evaluate the value of the functions in (a) and (b) for a giving x.
- Use *function* command to implement the composite Trapezoidal and Simpson's rules. The input arguments contain the integral interval $[a, b]$, integral function and stopping tolerance. The default tolerance is eps.