Euler-Maclaurin expansion

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Newton-Cotes quadrature formulae

For the approximation of

$$\int_a^b f(x)\,dx$$

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Let $x_k = a + k\,h,\ h = \frac{b-a}{n}$:

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

and

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

where

$$w_k := \int_a^b \ell_k(x)\, dx$$

are the weights of the quadrature.

Newton-Cotes: Trapezoid rule and Simpson's rule

$n = 1$, **Trapezoid**: $x_0 = a$, $x_1 = b$,

$$\int_a^b f(x)\,dx = \frac{b-a}{2}\,[f(a)+f(b)] + E_1(f)$$

error estimate

$$|E_1(f)| \leq M_2 \frac{(b-a)^3}{12}, \quad M_2 = \max_{x\in[a,b]} |f^{(2)}(x)|$$

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$n = 2$, **Simpson's**: $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$,

$$\int_a^b f(x)\,dx = \frac{b-a}{6}\left[f(a) + 4f(\frac{a+b}{2}) + f(b)\right] + E_2(f)$$

error estimate

$$|E_2(f)| \leq M_3 \frac{(b-a)^4}{196}, \quad M_3 = \max_{x\in[a,b]} |f^{(3)}(x)|$$

improved $E_2(f) = -\frac{(b-a)^5}{2880} f^{(4)}(\gamma), \qquad \gamma \in (a,b)$

Notation and Euler-Maclaurin expansion

Consider $[a, b] \subset \mathbf{R}$ and

$$I(f) := \int_a^b f(x)\, dx.$$

Suppose $h = \frac{b-a}{m}$

$$a = x_0 < x_1 \cdots < x_m = b, \quad x_i = a + i\, h$$

the composite trapezoid rule is

$$T(m) = T(h) = h\left(\frac{1}{2}f(x_0) + \sum_{i=1}^{m-1} f(x_i) + \frac{1}{2}f(x_m)\right),$$

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and we have seen that

$$|\mathcal{E}_1(f)| = |I(f) - T(h)| \leq \frac{(b-a)h^2}{12}\bar{M}_2, \qquad \bar{M}_2 = \max_{\xi\in[a,b]} |f''(\xi)|.$$

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Euler-Maclaurin: expansion in even powers of h

Suppose $f \in C^{2m}[a,b]$ then

$$I(f) - T(h) = \sum_{k=1}^{m-1} \frac{b_{2k}}{2k!}\,h^{2k}\,\left(f^{(2k-1)}(a) - f^{(2k-1)}(b)\right) - \frac{b_{2m}}{2m!}h^{2m}(b-a)f^{(2m)}(\eta),$$

and $\eta \in (a,b)$, b_k the Bernoulli numbers.

Romberg algorithm: extrapolation and composite trapezoid rule

Extrapolation:

$$
\begin{aligned}
I(f) - T(h) &= C_1 h^2 + C_2 h^4 + C_3 h^6 + \mathcal{O}(h^8) \\
I(f) - T(\frac{h}{2}) &= C_1 \frac{h^2}{4} + C_2 \frac{h^4}{16} + C_3 \frac{h^6}{64} + \mathcal{O}(h^8)
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$$I(f) - \frac{4T(\frac{h}{2}) - T(h)}{3} = -\frac{1}{4} C_2 h^4 - \frac{5}{16} C_3 h^6 + \mathcal{O}(h^8)$$

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repeat this trick k times to obtain the general formula:

$$T_k(h) = \frac{4^k\, T_{k-1}(\frac{h}{2}) - T_{k-1}(h)}{4^k - 1}, \quad k = 1, 2, 3, \ldots$$

Romberg matrix

Let $h_0 = b - a$ and $h_n = \frac{h_0}{2^n} = \frac{h_{n-1}}{2}$, $m = 2^n$ we can write the successively obtained approximations into a triangular matrix as follows

$$
\begin{array}{llll}
T_0(h_0) & & & \\
T_0(h_1) & T_1(h_0) & & \\
T_0(h_2) & T_1(h_1) & T_2(h_0) & \\
T_0(h_3) & T_1(h_2) & T_3(h_1) & T_4(h_0)
\end{array}
\qquad
\begin{array}{llll}
T_0(1) & & & \\
T_0(2) & T_1(1) & & \\
T_0(4) & T_1(2) & T_2(1) & \\
T_0(8) & T_1(4) & T_3(2) & T_4(1)
\end{array}
$$

and in yet another notation

$$
R(n,k) := T_k(h_{n-k}) = T_k(2^{n-k}), \qquad
\begin{array}{llll}
R(0,0) & & & \\
R(1,0) & R(1,1) & & \\
R(2,0) & R(2,1) & R(2,2) & \\
R(3,0) & R(3,1) & R(3,2) & R(3,3)
\end{array}
$$

The first column is the usual composite trapezium rule with more and more points, the other columns contain the approximations improved via extrapolation, the diagonal is supposed to get the best approximations provided f is smooth.

Romberg algorithm: recursive formulae

The first column is simply the composite trapezium rule were we half the step-size and fill inn more and more values of f. This gives:

$$R(n,0) = \frac{1}{2}R(n-1,0) + h_n \sum_{i=1}^{2^{(n-1)}} f(a + (2i-1)h_n).$$

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For the rest of the matrix, since $T_k(h) = \frac{4^k\, T_{k-1}(\frac{h}{2}) - T_{k-1}(h)}{4^k - 1}$, we have

$$R(n,k) = R(n,k-1) + \frac{1}{4^k-1}\big(R(n,k-1) - R(n-1,k-1)\big).$$

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$$R(n,k) = R(n,k-1) + \frac{1}{4^k-1}\big(R(n,k-1) - R(n-1,k-1)\big).$$

This gives automatically the error estimate:

$$E(n,k) := R(n,k) - R(n,k-1) = \frac{1}{4^k-1}\big(R(n,k-1) - R(n-1,k-1)\big).$$

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and $\eta \in (a, b)$, b_k the Bernoulli numbers.

Bernoulli polynomials

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Properties

1. $B_k(0) = B_k(1)$ for $k \geq 2$
2. $B_k(1-t) = (-1)^k B_k(t)$
3. $B_k(t) - B_k(0)$ does not have zeros in $(0,1)$ if k is even.

Bernoulli numbers $b_k := B_k(0)$
and (1) and (2) imply $b_k = 0$ for k odd and $k \geq 3$

Theorem

If $f : [a, b] \to \mathbb{R}$ is continuous and $g : [a, b] \to \mathbb{R}$ is integrable and nonnegative on (a, b).
Then $\exists\ \eta \in (a, b)$ such that

$$\int_a^b f(x)g(x)\mathrm{d}x = f(\eta) \int_a^b g(x)\mathrm{d}x.$$