Numerical Analysis

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with thanks to Endre Süli

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Newton–Cotes quadrature continued

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$$\int_a^b f(x)\,\mathrm{d}x = \int_{x_0}^{x_n} f(x)\,\mathrm{d}x = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)\,\mathrm{d}x$$

in which each $\displaystyle\int_{x_{i-1}}^{x_i} f(x)\,\mathrm{d}x$ is approximated by quadrature.

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Thus rather than increasing the degree of the polynomials to attain high accuracy, instead increase the number of intervals.

Trapezium Rule:

$$\int_{x_{i-1}}^{x_i} f(x)\,\mathrm{d}x = \frac{h}{2}[f(x_{i-1}) + f(x_i)] - \frac{h^3}{12} f''(\xi_i)$$

for some $\xi_i \in (x_{i-1}, x_i)$

Composite Trapezium Rule:

$$\int_{x_0}^{x_n} f(x)\,\mathrm{d}x = \sum_{i=1}^{n} \left[\frac{h}{2}[f(x_{i-1}) + f(x_i)] - \frac{h^3}{12} f''(\xi_i) \right]$$
$$= \frac{h}{2}\ [f(x_0) + 2f(x_1) + 2f(x_2) + \ldots + 2f(x_{n-1}) + f(x_n)] + e_h^{\mathsf{T}}$$

where $\xi_i \in (x_{i-1}, x_i)$ and $h = x_i - x_{i-1} = (x_n - x_0)/n = (b-a)/n$, and the error e_h^{T} is given by

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for some $\xi \in (a,b)$, using the Intermediate-Value Theorem n times (see Lecture 2: $\alpha f(\xi_i) + \beta f(\xi_{i+1}) = (\alpha+\beta)f(\xi)$ for some $\xi \in (\xi_i, \xi_{i+1})$)

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$$\sum_{i=1}^{n} f''(\xi_i) = 2f''(\xi^{[1]}) + \sum_{i=3}^{n} f''(\xi_i) = 3f''(\xi^{[2]}) + \sum_{i=4}^{n} f''(\xi_i) = \cdots = nf''(\xi^{[n]})$$

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Note that if we halve the stepsize h by introducing a new point half way between each current pair (x_{i-1}, x_i), the factor h^2 in the error will decrease by four.

Another composite rule: if $[a,b]=[x_0,x_{2n}]$,

$$\int_a^b f(x)\,\mathrm{d}x = \int_{x_0}^{x_{2n}} f(x)\,\mathrm{d}x = \sum_{i=1}^{n} \int_{x_{2i-2}}^{x_{2i}} f(x)\,\mathrm{d}x$$

in which each $\displaystyle\int_{x_{2i-2}}^{x_{2i}} f(x)\,\mathrm{d}x$ is approximated by quadrature.

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in which each $\displaystyle\int_{x_{2i-2}}^{x_{2i}} f(x)\,\mathrm{d}x$ is approximated by quadrature.

Simpson's Rule:

$$\int_{x_{2i-2}}^{x_{2i}} f(x)\,\mathrm{d}x = \frac{h}{3}[f(x_{2i-1}) + 4f(x_{2i-1}) + f(x_{2i})] - \frac{(2h)^5}{2880} f''''(\xi_i)$$

for some $\xi_i \in (x_{2i-2}, x_{2i})$.

Composite Simpson's Rule:

$$\int_{x_0}^{x_n} f(x)\,\mathrm{d}x = \sum_{i=1}^{n}\left[\frac{h}{3}[f(x_{2i-1}) + 4f(x_{2i-1}) + f(x_{2i})] - \frac{(2h)^5}{2880}f''''(\xi_i)\right]$$
$$= \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \dots$$
$$+ 2f(x_{2n-2}) + 4f(x_{2n-1}) + f(x_{2n})] + e_h^{\mathsf{S}}$$

where $\xi_i \in (x_{2i-2}, x_{2i})$ and $h = x_i - x_{i-1} = (x_{2n} - x_0)/2n = (b-a)/2n$, and the error e_h^{S} is given by

$$e_h^{\mathsf{S}} = -\frac{(2h)^5}{2880}\sum_{i=1}^{n} f''''(\xi_i) = -\frac{n(2h)^5}{2880}f''''(\xi) = -(b-a)\frac{h^4}{180}f''''(\xi)$$

for some $\xi \in (a,b)$, using the Intermediate-Value Theorem n times.

Composite Simpson's Rule:

$$\int_{x_0}^{x_n} f(x)\,\mathrm{d}x = \sum_{i=1}^{n}\left[\frac{h}{3}[f(x_{2i-1}) + 4f(x_{2i-1}) + f(x_{2i})] - \frac{(2h)^5}{2880}f''''(\xi_i)\right]$$
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for some $\xi \in (a,b)$, using the Intermediate-Value Theorem n times.

Note that if we halve the stepsize h by introducing a new point half way between each current pair (x_{i-1}, x_i), the factor h^4 in the error will decrease by sixteen.

Adaptive procedure: if S_h is the value given by Simpson's rule with a stepsize h, then

$$S_h - S_{\frac{1}{2}h} \approx \frac{15}{16} e_h^{\mathsf{S}}.$$

This suggests that if we wish to compute $\int_a^b f(x)\,\mathrm{d}x$ with an absolute error ϵ, we should compute the sequence $S_h, S_{\frac{1}{2}h}, S_{\frac{1}{4}h}, \ldots$ and stop when the difference, in absolute value, between two consecutive values is smaller than $15/16\epsilon$. That will ensure that (approximately) $|e_h^{\mathsf{S}}| \leq \epsilon$.

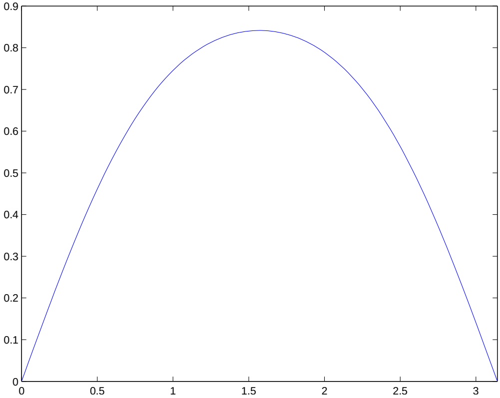
Sometimes much better accuracy may be obtained: for example, as might happen when computing Fourier coefficients, if f is periodic with period $b - a$ so that $f(a + x) = f(b + x)$ for all x.

Matlab:

```
% matlab
>> help adaptive_simpson
 ADAPTIVE_SIMPSON  Adaptive Simpson's rule.
    S = ADAPTIVE_SIMPSON(F,A,B,NMAX,TOL) computes an approximation
    to the integral of F on the interval [A,B]. It will take a
    maximum of NMAX steps and will attempt to determine the
    integral to a tolerance of TOL.

    The function uses an adaptive Simpson's rule, as described
    in lectures.
```

```
>> f = inline('sin(x)');
>> adaptive_simpson(f,0,pi,8,1.0e-7);
Step 1 integral is 2.0943951024, with error estimate 2.0944.
Step 2 integral is 2.0045597550, with error estimate 0.089835.
Step 3 integral is 2.0002691699, with error estimate 0.0042906.
Step 4 integral is 2.0000165910, with error estimate 0.00025258.
Step 5 integral is 2.0000010334, with error estimate 1.5558e-05.
Step 6 integral is 2.0000000645, with error estimate 9.6884e-07.
Successful termination at iteration 7:
The integral is 2.0000000040, with error estimate 6.0498e-08.
```




```
>> g = inline('sin(sin(x))');
>> fplot(g,[0,pi])
```

```
>> adaptive_simpson(g,0,pi,8,1.0e-7);
Step 1 integral is 1.7623727094, with error estimate 1.7624.
Step 2 integral is 1.8011896009, with error estimate 0.038817.
Step 3 integral is 1.7870879453, with error estimate 0.014102.
Step 4 integral is 1.7865214631, with error estimate 0.00056648.
Step 5 integral is 1.7864895607, with error estimate 3.1902e-05.
Step 6 integral is 1.7864876112, with error estimate 1.9495e-06.
Step 7 integral is 1.7864874900, with error estimate 1.2118e-07.
Successful termination at iteration 8:
The integral is 1.7864874825, with error estimate 7.5634e-09.
```