

Composite Numerical Integration

MATH 375 *Numerical Analysis*

J Robert Buchanan

Department of Mathematics

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Background

Remarks:

- ▶ The $(n + 1)$ -point Newton-Cotes formulas with small n are not suitable for integrating over long intervals due to large values of the truncation error.

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- ▶ The $(n + 1)$ -point Newton-Cotes formulas with small n are not suitable for integrating over long intervals due to large values of the truncation error.
- ▶ If we choose a large n , the coefficients of the Newton-Cotes formulas are difficult to determine.
- ▶ The Newton-Cotes formulas are based on Lagrange interpolating polynomials with equally spaced nodes. These polynomials can have large oscillations between the nodes.

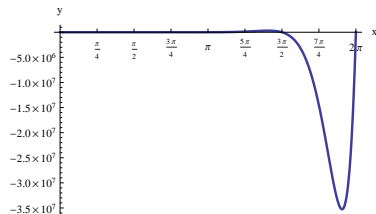
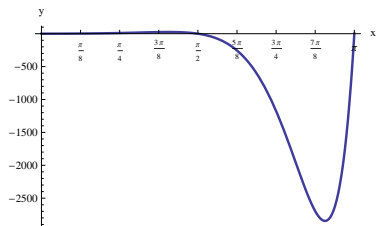
Test Case

Throughout this presentation we will use the following definite integral to evaluate the performance of the various approximations.

$$\begin{aligned}\int_0^{2\pi} e^{3x} \sin 2x \, dx &= \left[\frac{1}{13} e^{3x} (3 \sin 2x - 2 \cos 2x) \right]_{x=0}^{x=2\pi} \\ &= \frac{2}{13} (1 - e^{6\pi}) \\ &\approx -2.36235 \times 10^7\end{aligned}$$

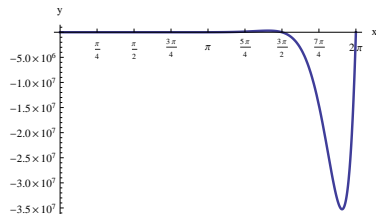
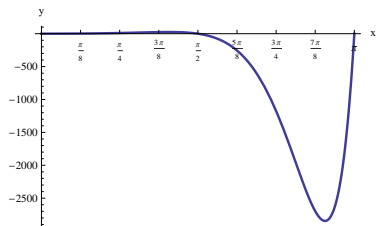
Graphs

Considering the graphs of the integrand shown below, do you anticipate any difficulties using the Newton-Cotes formulas to approximate the definite integral?



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The graph of the left covers $0 \leq x \leq \pi$ while the graph on the right is for the interval $0 \leq x \leq 2\pi$.

Common Quadrature Formulas (1 of 4)

Closed Newton-Cotes:

Trapezoidal Rule

$$\int_a^b f(x) dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12}f''(z).$$

Simpson's Rule

$$\int_{x_0}^{x_2} f(x) dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90}f^{(4)}(z)$$

Common Quadrature Formulas (2 of 4)

Closed Newton-Cotes:

Simpson's 3/8 Rule

$$\int_{x_0}^{x_3} f(x) dx = \frac{3h}{8} [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80} f^{(4)}(z).$$

Closed Newton-Cotes $n = 4$

$$\begin{aligned} \int_{x_0}^{x_4} f(x) dx &= \frac{2h}{45} [7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)] \\ &\quad - \frac{8h^7}{945} f^{(6)}(z) \end{aligned}$$

Common Quadrature Formulas (3 of 4)

Open Newton-Cotes:

Midpoint Rule

$$\int_{x_{-1}}^{x_1} f(x) dx = 2hf(x_0) + \frac{h^3}{3}f''(z)$$

Open Newton-Cotes $n = 1$

$$\int_{x_{-1}}^{x_2} f(x) dx = \frac{3h}{2} [f(x_0) + f(x_1)] + \frac{3h^3}{4}f''(z)$$

Common Quadrature Formulas (3 of 4)

Open Newton-Cotes:

Open Newton-Cotes $n = 2$

$$\int_{x_{-1}}^{x_3} f(x) dx = \frac{4h}{3} [2f(x_0) - f(x_1) + 2f(x_2)] + \frac{14h^5}{45} f^{(4)}(z)$$

Open Newton-Cotes $n = 3$

$$\int_{x_{-1}}^{x_4} f(x) dx = \frac{5h}{24} [11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)] + \frac{95h^5}{144} f^{(4)}(z)$$

Performance (1 of 2)

Closed Newton-Cotes:

Method	Approx.	Abs. Err.	Err. Bound
Trapezoidal	0.0	2.36235×10^7	3.80888×10^{10}
Simpson's	0.0	2.36235×10^7	6.26536×10^{10}
Simpson's 3/8	584030.0	2.42076×10^7	2.78461×10^{10}
Closed N-C $n = 4$	0.0	2.36235×10^7	8.66687×10^9

Performance (2 of 2)

Open Newton-Cotes:

Method	Approx.	Abs. Err.	Err. Bound
Midpoint	0.0	2.36235×10^7	1.90444×10^{10}
Open N-C $n = 1$	778707.0	2.44022×10^7	1.26963×10^{10}
Open N-C $n = 2$	0.0	2.36235×10^7	5.48219×10^{10}
Open N-C $n = 3$	-5.97228×10^6	1.76513×10^7	3.80934×10^9

Subdivision

Recall the property of the definite integral:

$$\int_a^b f(x) dx = \int_a^c f(x) dx + \int_c^b f(x) dx$$

Use this property and Simpson's Rule to evaluate the test case again.

$$\int_0^{2\pi} e^{3x} \sin 2x dx = \int_0^{\pi} e^{3x} \sin 2x dx + \int_{\pi}^{2\pi} e^{3x} \sin 2x dx$$

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Since we must evaluate the first integrand at $x = 0$, $\pi/2$, and π and the second integrand at $x = \pi$, $3\pi/2$, and 2π , then

$$\int_0^{2\pi} e^{3x} \sin 2x dx \approx 0 + 0 = 0.$$

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$$\int_0^{2\pi} e^{3x} \sin 2x dx \approx 0 + 0 = 0.$$

Question: what is happening to our numerical integration formulas in this example?

Further Subdivision

If $f(x) = e^{3x} \sin 2x$ then

$$\begin{aligned} \int_0^{2\pi} f(x) dx &= \int_0^{\pi/2} f(x) dx + \int_{\pi/2}^{\pi} f(x) dx \\ &\quad + \int_{\pi}^{3\pi/2} f(x) dx + \int_{3\pi/2}^{2\pi} f(x) dx \end{aligned}$$

and applying Simpson's Rule to each of the definite integrals on the right-hand side yields

$$\begin{aligned} \int_0^{2\pi} f(x) dx &\approx 11.0487 - 1229.92 + 136912 - 1.52407 \times 10^7 \\ &\approx -1.5105 \times 10^7 \end{aligned}$$

which has an absolute error of 8.51854×10^6

Developing the Composite Simpson's Rule (1 of 2)

Given $\int_a^b f(x) dx$, let $m = 2n$ and partition $[a, b]$ into m subintervals.

Then

$$\int_a^b f(x) dx = \sum_{j=1}^n \int_{x_{2j-2}}^{x_{2j}} f(x) dx.$$

Developing the Composite Simpson's Rule (2 of 2)

Apply Simpson's Rule on each consecutive pair of subintervals.

$$h = \frac{b-a}{2n}$$
$$x_j = a + jh \quad \text{for } j = 1, 2, \dots, m$$

Then

$$\int_a^b f(x) dx = \sum_{j=1}^n \left[\frac{h}{3} (f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})) - \underbrace{\frac{h^5}{90} f^{(4)}(z_j)}_{E(f)_j} \right]$$

where $x_{2j-2} \leq z_j \leq x_{2j}$ for $j = 1, 2, \dots, n$.

Simplify Composite Simpson's Rule (1 of 3)

Note: the node x_{2j} can be thought of as the right-hand node of the $j - 1$ th subinterval and also as the left-hand node of the j th subinterval for $j = 1, 2, \dots, n - 1$.

$$\begin{aligned}\int_a^b f(x) dx &= \sum_{j=1}^n \int_{x_{2j-2}}^{x_{2j}} f(x) dx \\ &= \sum_{j=1}^n \left[\frac{h}{3} (f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})) - E(f)_j \right] \\ &= \frac{h}{3} \left[\sum_{j=1}^n f(x_{2j-2}) + 4 \sum_{j=1}^n f(x_{2j-1}) + \sum_{j=1}^n f(x_{2j}) \right] \\ &\quad - \underbrace{\sum_{j=1}^n E(f)_j}_{E(f)}\end{aligned}$$

Simplify Composite Simpson's Rule (2 of 3)

Pull out the first term of the first summation and the last term of the last summation.

$$\int_a^b f(x) dx = \frac{h}{3} \left[f(x_0) + \sum_{j=2}^n f(x_{2j-2}) + 4 \sum_{j=1}^n f(x_{2j-1}) + \sum_{j=1}^{n-1} f(x_{2j}) + f(x_{2n}) \right] - E(f)$$

Now re-index the first summation.

Simplify Composite Simpson's Rule (3 of 3)

$$\begin{aligned}\int_a^b f(x) dx &= \frac{h}{3} \left[f(x_0) + \sum_{j=2}^n f(x_{2j-2}) + 4 \sum_{j=1}^n f(x_{2j-1}) \right. \\ &\quad \left. + \sum_{j=1}^{n-1} f(x_{2j}) + f(x_{2n}) \right] - E(f) \\ &= \frac{h}{3} \left[f(x_0) + \sum_{j=1}^{n-1} f(x_{2j}) + 4 \sum_{j=1}^n f(x_{2j-1}) \right. \\ &\quad \left. + \sum_{j=1}^{n-1} f(x_{2j}) + f(x_{2n}) \right] - E(f) \\ &= \frac{h}{3} \left[f(x_0) + 2 \sum_{j=1}^{n-1} f(x_{2j}) + 4 \sum_{j=1}^n f(x_{2j-1}) + f(x_{2n}) \right] - E(f)\end{aligned}$$

Error Term (1 of 3)

We can express the truncation error for the Composite Simpson's Rule as

$$E(f) = -\frac{h^5}{90} \sum_{j=1}^n f^{(4)}(z_j).$$

Error Term (1 of 3)

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- ▶ If $f \in C^4[a, b]$ then by the Extreme Value Theorem

$$\min_{a \leq x \leq b} f^{(4)}(x) \leq f^{(4)}(z_j) \leq \max_{a \leq x \leq b} f^{(4)}(x)$$

for $j = 1, 2, \dots, n$.

- ▶ Summing over $j = 1, 2, \dots, n$:

$$\sum_{j=1}^n \min_{a \leq x \leq b} f^{(4)}(x) \leq \sum_{j=1}^n f^{(4)}(z_j) \leq \sum_{j=1}^n \max_{a \leq x \leq b} f^{(4)}(x)$$

Error Term (2 of 3)

$$\sum_{j=1}^n \min_{a \leq x \leq b} f^{(4)}(x) \leq \sum_{j=1}^n f^{(4)}(z_j) \leq \sum_{j=1}^n \max_{a \leq x \leq b} f^{(4)}(x)$$

$$n \left(\min_{a \leq x \leq b} f^{(4)}(x) \right) \leq \sum_{j=1}^n f^{(4)}(z_j) \leq n \left(\max_{a \leq x \leq b} f^{(4)}(x) \right)$$

$$\min_{a \leq x \leq b} f^{(4)}(x) \leq \frac{1}{n} \sum_{j=1}^n f^{(4)}(z_j) \leq \max_{a \leq x \leq b} f^{(4)}(x)$$

Error Term (3 of 3)

Since

$$\min_{a \leq x \leq b} f^{(4)}(x) \leq \frac{1}{n} \sum_{j=1}^n f^{(4)}(z_j) \leq \max_{a \leq x \leq b} f^{(4)}(x)$$

according to the Intermediate Value Theorem there exists $a \leq \mu \leq b$ such that

$$f^{(4)}(\mu) = \frac{1}{n} \sum_{j=1}^n f^{(4)}(z_j).$$

Error Term (3 of 3)

Since

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$$f^{(4)}(\mu) = \frac{1}{n} \sum_{j=1}^n f^{(4)}(z_j).$$

Thus we may express the truncation error as

$$\begin{aligned} E(f) &= -\frac{h^5}{90} n f^{(4)}(\mu) = -\frac{h^5}{90} \left(\frac{b-a}{2h} \right) f^{(4)}(\mu) \\ &= -\frac{b-a}{180} h^4 f^{(4)}(\mu). \end{aligned}$$

Composite Simpson's Rule

Theorem

Let $f \in C^4[a, b]$, $n \in \mathbb{N}$ be even, $h = (b - a)/n$, and $x_j = a + jh$ for $j = 0, 1, \dots, n$. There exists $\mu \in (a, b)$ for which the **Composite Simpson's Rule** for n subintervals can be written with its error term as

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

Composite Simpson's Rule (Example $n = 128$)

$$\int_0^{2\pi} e^{3x} \sin 2x \, dx \approx -2.36233 \times 10^7$$

Absolute error ≈ 227.661
Error bound ≈ 3734.45

Composite Simpson's Rule (Example $n = 512$)

$$\int_0^{2\pi} e^{3x} \sin 2x \, dx \approx -2.36235 \times 10^7$$

$$\text{Absolute error} \approx 0.889943$$

$$\text{Error bound} \approx 14.5877$$

Composite Trapezoidal Rule

Theorem

Let $f \in \mathcal{C}^2[a, b]$, $n \in \mathbb{N}$, $h = (b - a)/n$, and $x_j = a + jh$ for $j = 0, 1, \dots, n$. There exists $\mu \in (a, b)$ for which the **Composite Trapezoidal Rule** for n subintervals can be written with its error term as

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

Composite Trapezoidal Rule (Example $n = 256$)

$$\int_0^{2\pi} e^{3x} \sin 2x \, dx \approx -2.36081 \times 10^7$$

Absolute error ≈ 15413.0

Error bound ≈ 581190.0

Composite Trapezoidal Rule (Example $n = 1024$)

$$\int_0^{2\pi} e^{3x} \sin 2x \, dx \approx -2.36226 \times 10^7$$

$$\text{Absolute error} \approx 963.519$$

$$\text{Error bound} \approx 36324.3$$

Composite Midpoint Rule

Theorem

Let $f \in \mathcal{C}^2[a, b]$, $n \in \mathbb{N}$ be even, $h = (b - a)/(n + 2)$, and $x_j = a + (j + 1)h$ for $j = -1, 0, \dots, n + 1$. There exists $\mu \in (a, b)$ for which the **Composite Midpoint Rule** for $n + 2$ subintervals can be written with its error term as

$$\int_a^b f(x) dx = 2h \sum_{j=0}^{n/2} f(x_{2j}) + \frac{b-a}{6} h^2 f''(\mu).$$

Composite Midpoint Rule (Example $n = 1024$)

$$\int_0^{2\pi} e^{3x} \sin 2x \, dx \approx -2.36254 \times 10^7$$

$$\text{Absolute error} \approx 1919.37$$

$$\text{Error bound} \approx 72365.7$$

Composite Midpoint Rule (Example $n = 4096$)

$$\int_0^{2\pi} e^{3x} \sin 2x \, dx \approx -2.36236 \times 10^7$$

$$\text{Absolute error} \approx 120.323$$

$$\text{Error bound} \approx 4536.11$$

Estimating the Number of Subdivisions

Consider the task of estimating $\int_0^{10} e^x dx$ with an absolute error of $\epsilon \leq 10^{-6}$.

How many subdivisions of $[0, 10]$ are required for the

- ▶ Composite Simpson's Rule?
- ▶ Composite Trapezoidal Rule?
- ▶ Composite Midpoint Rule?

Composite Simpson's Rule Estimate of n

$$\begin{aligned} E(f) &\leq 10^{-6} \\ \left| \frac{b-a}{180} h^4 f^{(4)}(\mu) \right| &\leq 10^{-6} \\ \left| \frac{10}{180} \left(\frac{10}{n} \right)^4 e^{\mu} \right| &\leq 10^{-6} \\ \frac{10000}{n^4} &\leq 18e^{-10} \times 10^{-6} \\ n^4 &\geq \frac{10^{10}}{18} e^{10} \\ n &\geq \sqrt[4]{\frac{10^{10}}{18} e^{10}} \approx 1870.33 \\ n &\geq 1872 \end{aligned}$$

since n must be even in the Composite Simpson's Rule.

Composite Trapezoidal Rule Estimate of n

$$\begin{aligned} E(f) &\leq 10^{-6} \\ \left| \frac{b-a}{12} h^2 f''(\mu) \right| &\leq 10^{-6} \\ \left| \frac{10}{12} \left(\frac{10}{n} \right)^2 e^\mu \right| &\leq 10^{-6} \\ \frac{100}{n^2} &\leq 12e^{-10} \times 10^{-7} \\ n^2 &\geq \frac{10^9}{12} e^{10} \\ n &\geq \sqrt{\frac{10^9}{12} e^{10}} \approx 1.354820 \times 10^6 \\ n &\geq 1354821 \end{aligned}$$

Composite Midpoint Rule Estimate of n

$$\begin{aligned} E(f) &\leq 10^{-6} \\ \left| \frac{b-a}{6} h^2 f''(\mu) \right| &\leq 10^{-6} \\ \left| \frac{10}{6} \left(\frac{10}{n} \right)^2 e^\mu \right| &\leq 10^{-6} \\ \frac{100}{n^2} &\leq 6e^{-10} \times 10^{-7} \\ n^2 &\geq \frac{10^9}{6} e^{10} \\ n &\geq \sqrt{\frac{10^9}{6} e^{10}} \approx 1.916006 \times 10^6 \\ n &\geq 1916006 \end{aligned}$$

Summary

Composite Simpson's Rule (n even):

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

Composite Trapezoidal Rule:

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Composite Midpoint Rule (n even):

$$\int_a^b f(x) dx = 2h \sum_{j=0}^{n/2} f(x_{2j}) + \frac{b-a}{6} h^2 f''(\mu).$$

Round-Off Error

Every composite quadrature method requires that we evaluate $f(x_i)$.

$$\underbrace{f(x_i)}_{\text{true value}} = \underbrace{\hat{f}(x_i)}_{\text{numerical value}} + \underbrace{e_i}_{\text{round-off error}}$$

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Question: if we form n evaluations of $f(x_i)$ how does the round-off error accumulate?

Round-Off Error for Composite Simpson's Rule (1 of 2)

$$e(h) = \frac{h}{3} \left[e_0 + 2 \sum_{j=1}^{n-1} e_{2j} + 4 \sum_{j=1}^n e_{2j-1} + e_{2n} \right]$$

$$|e(h)| \leq \frac{h}{3} \left[|e_0| + 2 \sum_{j=1}^{n-1} |e_{2j}| + 4 \sum_{j=1}^n |e_{2j-1}| + |e_{2n}| \right]$$

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$$|e(h)| \leq \frac{h}{3} \left[|e_0| + 2 \sum_{j=1}^{n-1} |e_{2j}| + 4 \sum_{j=1}^n |e_{2j-1}| + |e_{2n}| \right]$$

Suppose all the round-off errors are bounded by ϵ .

$$|e(h)| \leq \frac{h}{3} \left[\epsilon + 2 \sum_{j=1}^{n-1} \epsilon + 4 \sum_{j=1}^n \epsilon + \epsilon \right]$$

Round-Off Error for Composite Simpson's Rule (2 of 2)

$$\begin{aligned} |e(h)| &\leq \frac{h}{3} \left[\epsilon + 2 \sum_{j=1}^{n-1} \epsilon + 4 \sum_{j=1}^n \epsilon + \epsilon \right] \\ &= \frac{h}{3} (1 + 2(n-1) + 4(n) + 1) \epsilon \\ &= 2hn\epsilon \\ &= (b-a)\epsilon \end{aligned}$$

Round-Off Error for Composite Simpson's Rule (2 of 2)

$$\begin{aligned} |e(h)| &\leq \frac{h}{3} \left[\epsilon + 2 \sum_{j=1}^{n-1} \epsilon + 4 \sum_{j=1}^n \epsilon + \epsilon \right] \\ &= \frac{h}{3} (1 + 2(n-1) + 4(n) + 1) \epsilon \\ &= 2hn\epsilon \\ &= (b-a)\epsilon \end{aligned}$$

Remark: the Composite Simpson's Rule is stable with respect to round-off error.

Round-Off Error

Remarks:

- ▶ The composite quadrature formulas are stable with respect to round-off error (we can make h as small as we like).
- ▶ The numerical differentiation formulas were unstable with respect to round-off error.

Homework

- ▶ Read Section 4.4
- ▶ Exercises: 1ad, 3ad, 5ad, 11, 17, 21