Numerical Analysis

SMIE SYSU

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Outline

- May 27
- June 3

Numerical Differentiation and Integration S1

- Computational calculus: compute derivatives and integrals of functions $y=f(x)$.
- Two main methods for the problem:

1. Symbolic computing
2. Numerical computing (major topic in this chapter)

Numerical Differentiation and Integration S2

- Symbolic computing

If a function y=f(x) is written in terms of elementary functions, e.g. $f(x) = \sin^3(x^{\tan x} \cosh x)$ both of its derivatives and antiderivatives (indefinite integrals) can be expressed in terms of elementary functions.

- Numerical computing (major topic in this chapter)

The function is given as a tabulated list, e.g., $\{\{t_1,T_1\},\ldots,\{t_n, T_n\}\}$ of time/temperature pairs. The output of both derivatives and antiderivatives can be the form of the numerical pairs. In this case, the symbolic computing is not applicable. The numerical computing is a good choice.

Numerical Differentiation

- Finite difference formulas
- Rounding error
- Extrapolation
- Symbolic differentiation and integration

Finite difference formulas S1

By definition, the derivative of $f(x)$ at a value x is

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}, \tag{5.1}$$

provided that the limit exists.

Taylor's Theorem says that if f is twice continuously differentiable, then

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(c), \tag{5.2}$$

where c is between x and $x + h$.

Finite difference formulas S2

Two-point forward-difference formula

$$f'(x) = \boxed{\frac{f(x+h) - f(x)}{h}} - \frac{h}{2} f''(c), \tag{5.3}$$

where c is between x and $x + h$.

The quotient will closely approximate the derivative if h is small.

We use (5.3) by computing the approximation

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \tag{5.4}$$

and treating the last term in (5.3) as error.

The first-order method for approximating the first derivative.

In general, if the error is $O(h^n)$, we call the formula an **order** n approximation.

Finite difference formulas S3

- Example

Use the two-point forward-difference formula with $h = 0.1$ to approximate the derivative of $f(x) = 1/x$ at $x = 2$.

The two-point forward-difference formula (5.4) evaluates to

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} = \frac{\frac{1}{2.1} - \frac{1}{2}}{0.1} \approx -0.2381.$$

The difference between this approximation and the correct derivative $f'(x) = -x^{-2}$ at $x = 2$ is the error

$$-0.2381 - (-0.2500) = 0.0119.$$

Compare this to the error predicted by the formula, which is $hf''(c)/2$ for some c between 2 and 2.1. Since $f''(x) = 2x^{-3}$, the error must be between

$$(0.1)2^{-3} \approx 0.0125 \quad \text{and} \quad (0.1)(2.1)^{-3} \approx 0.0108,$$

which is consistent with our result. However, this information is usually not available. ◀

Finite difference formulas S4

A second-order formula can be developed by a more advanced strategy. According to Taylor's Theorem, if f is three times continuously differentiable, then

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(c_1)$$

and

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(c_2),$$

where $x - h < c_2 < x < c_1 < x + h$. Subtracting the two equations gives the following three-point formula with an explicit error term:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} \boxed{- \frac{h^2}{12}f'''(c_1) - \frac{h^2}{12}f'''(c_2).} \tag{5.5}$$

How to measure this error?

Finite difference formulas S5

- Theorem

Generalized Intermediate Value Theorem. Let f be a continuous function on the interval $[a, b]$. Let $x_1, \ldots, x_n$ be points in $[a, b]$, and $a_1, \ldots, a_n > 0$. Then there exists a number c between a and b such that

$$(a_1 + \cdots + a_n) f(c) = a_1 f(x_1) + \cdots + a_n f(x_n). \tag{5.6}$$

Proof. Let $f(x_i)$ equal the minimum and $f(x_j)$ the maximum of the n function values. Then

$$a_1 f(x_i) + \cdots + a_n f(x_i) \le a_1 f(x_1) + \cdots + a_n f(x_n) \le a_1 f(x_j) + \cdots + a_n f(x_j)$$

implies that

$$f(x_i) \le \frac{a_1 f(x_1) + \cdots + a_n f(x_n)}{a_1 + \cdots + a_n} \le f(x_j).$$

By the Intermediate Value Theorem, there is a number c between x_i and x_j such that

$$f(c) = \frac{a_1 f(x_1) + \cdots + a_n f(x_n)}{a_1 + \cdots + a_n},$$

and (5.6) is satisfied. ❐

Finite difference formulas S6

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} \boxed{- \frac{h^2}{12} f'''(c_1) - \frac{h^2}{12} f'''(c_2).}$$

$$\boxed{(a_1 + \cdots + a_n) f(c) = a_1 f(x_1) + \cdots + a_n f(x_n)}$$

Three-point centered-difference formula

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} \boxed{- \frac{h^2}{6} f'''(c),} \tag{5.7}$$

where $x - h < c < x + h$.

Finite difference formulas S7

- Example

Use the three-point centered-difference formula with $h = 0.1$ to approximate the derivative of $f(x) = 1/x$ at $x = 2$.

The three-point centered-difference formula evaluates to

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} = \frac{\frac{1}{2.1} - \frac{1}{1.9}}{0.2} \approx -0.2506.$$

The error is 0.0006, an improvement on the two-point forward-difference formula in Example 5.1. ◀

The error for the two-point forward-difference formula is 0.0119.

Finite difference formulas S8

Approximation formulas for higher derivatives can be obtained in the same way. For example, the Taylor expansions

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(\mathrm{iv})}(c_1)$$

and

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(\mathrm{iv})}(c_2),$$

where $x - h < c_2 < x < c_1 < x + h$ can be added together to eliminate the first derivative terms to get

$$f(x+h) + f(x-h) - 2f(x) = h^2 f''(x) + \frac{h^4}{24}f^{(\mathrm{iv})}(c_1) + \frac{h^4}{24}f^{(\mathrm{iv})}(c_2).$$

Three-point centered-difference formula for second derivative

$$f''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} - \frac{h^2}{12}f^{(\mathrm{iv})}(c) \qquad (5.8)$$

for some c between $x - h$ and $x + h$.

Rounding error S1

- Example

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(c),$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(c),$$

Approximate the derivative of $f(x) = e^x$ at $x = 0$.

The two-point formula (5.4) gives

$$f'(x) \approx \frac{e^{x+h} - e^x}{h}, \tag{5.9}$$

and the three-point formula (5.7) yields

$$f'(x) \approx \frac{e^{x+h} - e^{x-h}}{2h}. \tag{5.10}$$

Rounding error S2

- Example (cont...)

The results of these formulas for $x = 0$ and a wide range of increment size h, along with errors compared with the correct value $e^0 = 1$, are given in the following table:

h	formula (5.9)	error	formula (5.10)	error
10^{-1}	1.05170918075648	−0.05170918075648	1.00166750019844	−0.00166750019844
10^{-2}	1.00501670841679	−0.00501670841679	1.00001666674999	−0.00001666674999
10^{-3}	1.00050016670838	−0.00050016670838	1.00000016666668	−0.00000016666668
10^{-4}	1.00005000166714	−0.00005000166714	1.00000000166689	−0.00000000166689
10^{-5}	1.00000500000696	−0.00000500000696	1.00000000001210	−0.00000000001210
10^{-6}	1.00000049996218	−0.00000049996218	0.99999999997324	0.00000000002676
10^{-7}	1.00000004943368	−0.00000004943368	0.99999999947364	0.00000000052636
10^{-8}	0.99999999392253	0.00000000607747	0.99999999392253	0.00000000607747
10^{-9}	1.00000008274037	−0.00000008274037	1.00000002722922	−0.00000002722922

Loss of significance

Rounding error S3

Denote the floating point version of the input $f(x+h)$ by $\hat{f}(x+h)$, which will differ from the correct value $f(x+h)$ by a number on the order of machine epsilon in relative terms.

Since $\hat{f}(x+h) = f(x+h) + \epsilon_1$ and $\hat{f}(x-h) = f(x-h) + \epsilon_2$, where $|\epsilon_1|, |\epsilon_2| \approx \epsilon_{\text{mach}}$, the difference between the correct $f'(x)$ and the machine version of the three-point centered-difference formula (5.7) is

$$
\begin{aligned}
f'(x)_{\text{correct}} - f'(x)_{\text{machine}} &= f'(x) - \frac{\hat{f}(x+h) - \hat{f}(x-h)}{2h} \\
&= f'(x) - \frac{f(x+h) + \epsilon_1 - (f(x-h) + \epsilon_2)}{2h} \\
&= \left(f'(x) - \frac{f(x+h) - f(x-h)}{2h} \right) + \frac{\epsilon_2 - \epsilon_1}{2h} \\
&= \underbrace{\boxed{\left(f'(x)_{\text{correct}} - f'(x)_{\text{formula}} \right)}}_{\text{Truncation error}} + \underbrace{\boxed{\text{error}_{\text{rounding}}.}}_{\text{Rounding error}}
\end{aligned}
$$

Total error

Rounding error S4

The rounding error has absolute value

$$\left|\frac{\epsilon_2 - \epsilon_1}{2h}\right| \le \frac{2\epsilon_{\text{mach}}}{2h} = \frac{\epsilon_{\text{mach}}}{h},$$

where ϵ_{mach} represents machine epsilon. Therefore, the absolute value of the error of the machine approximation of $f'(x)$ is bounded above by

$$E(h) \equiv \frac{h^2}{6} f'''(c) + \frac{\epsilon_{\text{mach}}}{h}, \tag{5.11}$$

where $x - h < c < x + h$. Previously we had considered only the first term of the error, the mathematical error. The preceding table forces us to consider the loss of significance term as well.

Because there are two terms in the absolute error, how to find the best h that minimizes the solution error?

Rounding error S5

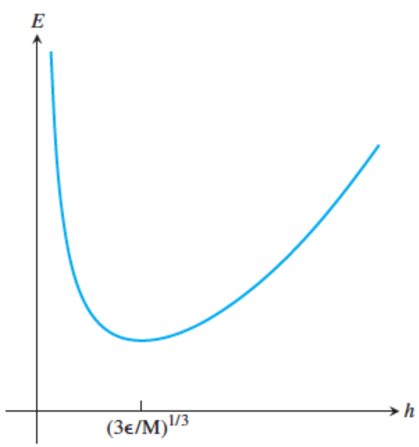
It is instructive to plot the function $E(h)$, shown in Figure 5.1. The minimum of $E(h)$ occurs at the solution of

$$0 = E'(h) = -\frac{\epsilon_{\text{mach}}}{h^2} + \frac{M}{3}h, \qquad (5.12)$$

where we have approximated $|f'''(c)| \approx |f'''(x)|$ by M. Solving (5.12) yields

$$h = (3\epsilon_{\text{mach}}/M)^{1/3}$$

for the increment size h that gives smallest overall error, including the effects of computer rounding. In double precision, this is approximately $\epsilon_{\text{mach}}^{1/3} \approx 10^{-5}$, consistent with the table.



The main message is that the three-point centered difference formula will improve in accuracy as h is decreased until h becomes about the size of the cube root of machine epsilon. As h drops below this size, the error may begin increasing again.

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(c),$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(c),$$

Extrapolation S1

Assume that we are presented with an order n formula $F(h)$ for approximating a given quantity Q. The order means that

The formula depends on h instead of on x.

$$Q \approx F(h) + Kh^n,$$

where K is roughly constant over the range of h in which we are interested. A relevant example is

$$\approx f'''(x)/6$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \boxed{\frac{f'''(c_h)}{6}} h^2, \tag{5.13}$$

In a case like this, a little bit of algebra can be used to leverage an order n formula into one of higher order. Because we know the order of the formula $F(h)$ is n, if we apply the formula again with $h/2$ instead of h, our error should be reduced from a constant times h^n to a constant times $(h/2)^n$, or reduced by a factor of 2^n. In other words, we expect

$$Q - F(h/2) \approx \frac{1}{2^n}(Q - F(h)). \tag{5.14}$$

We are relying on the assumption that K is roughly constant.

Extrapolation S2

Extrapolation for order n formula

$$Q \approx \frac{2^n F(h/2) - F(h)}{2^n - 1}. \tag{5.15}$$

This is the **extrapolation** formula for $F(h)$. Extrapolation, sometimes called **Richardson extrapolation**, typically gives a higher-order approximation of Q than $F(h)$. To understand why, assume that the nth-order formula $F_n(h)$ can be written

$$Q = F_n(h) + Kh^n + O(h^{n+1}).$$

Then cutting h in half yields $Q = F_n(h/2) + K\frac{h^n}{2^n} + O(h^{n+1})$,

and the extrapolated version, which we call $F_{n+1}(h)$, will satisfy

$$\begin{aligned} F_{n+1}(h) &= \frac{2^n F_n(h/2) - F_n(h)}{2^n - 1} \\ &= \frac{2^n(Q - Kh^n/2^n - O(h^{n+1})) - (Q - Kh^n - O(h^{n+1}))}{2^n - 1} \\ &= Q + \frac{-Kh^n + Kh^n + O(h^{n+1})}{2^n - 1} = Q + O(h^{n+1}). \end{aligned}$$

Therefore, $F_{n+1}(h)$ is (at least) an order $n+1$ formula for approximating the quantity Q.

Extrapolation S3

- Example

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f'''(c_h)}{6}h^2, \tag{5.13}$$

Apply extrapolation to formula (5.13).

We start with the second-order centered-difference formula $F_2(h)$ for the derivative $f'(x)$. The extrapolation formula (5.15) gives a new formula for $f'(x)$ as

Find the error in (5.16), 5 mins

$$\begin{aligned} F_4(x) &= \frac{2^2 F_2(h/2) - F_2(h)}{2^2 - 1} \\ &= \left[4\frac{f(x+h/2) - f(x-h/2)}{h} - \frac{f(x+h) - f(x-h)}{2h} \right] \Big/ 3 \\ &= \frac{f(x-h) - 8f(x-h/2) + 8f(x+h/2) - f(x+h)}{6h}. \end{aligned} \tag{5.16}$$

This is a five-point centered-difference formula. The previous argument guarantees that this formula is of order at least three, but it turns out to have order four, because the order three error terms cancel out. In fact, since $F_4(h) = F_4(-h)$ by inspection, the error must be the same for h as for $-h$. Therefore, the error terms can be even powers of h only. ◀

$$Q \approx F(h) + Kh^n$$

Extrapolation S3

- Example

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f'''(c_h)}{6}h^2, \qquad (5.13)$$

Apply extrapolation to formula (5.13).

We start with the second-order centered-difference formula $F_2(h)$ for the derivative $f'(x)$. The extrapolation formula (5.15) gives a new formula for $f'(x)$ as

$$\begin{aligned} \cancel{F_4(x)}\ F_4(h) &= \frac{2^2 F_2(h/2) - F_2(h)}{2^2 - 1} \\ &= \left[4\frac{f(x+h/2) - f(x-h/2)}{h} - \frac{f(x+h) - f(x-h)}{2h} \right] \bigg/ 3 \\ &= \frac{f(x-h) - 8f(x-h/2) + 8f(x+h/2) - f(x+h)}{6h}. \end{aligned} \qquad (5.16)$$

This is a five-point centered-difference formula. The previous argument guarantees that this formula is of order at least three, but it turns out to have order four, because the order three error terms cancel out. In fact, since $F_4(h) = F_4(-h)$ by inspection, the error must be the same for h as for $-h$. Therefore, the error terms can be even powers of h only. ◀

$$Q \approx F(h) + Kh^n$$

Extrapolation S4

- Example

$$f''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} - \frac{h^2}{12} f^{(\text{iv})}(c) \qquad (5.8)$$

Apply extrapolation to the second derivative formula (5.8).

Again, the method is second order, so the extrapolation formula (5.15) is used with $n = 2$. The extrapolated formula is

$$\cancel{F_4(x)} = \frac{2^2 F_2(h/2) - F_2(h)}{2^2 - 1}$$

$$F_4(h)$$

$$= \left[4 \frac{f(x+h/2) - 2f(x) + f(x-h/2)}{h^2/4} - \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \right] \Big/ 3$$

$$= \frac{-f(x-h) + 16f(x-h/2) - 30f(x) + 16f(x+h/2) - f(x+h)}{3h^2}.$$

The new method for approximating second derivatives is fourth order, for the same reason as the previous example. ◀

Symbolic differentiation and integration S1

- The Matlab Symbolic Toolbox contains commands for obtaining the symbolic derivative of symbolically written functions.
- Differentiation uses the Matlab symbolic command diff
- Integration uses the Matlab symbolic command int

```
>> syms x;
>> f=sin(3*x);
>> f1=diff(f)

f1=

3*cos(3*x)
```

```
>>f3=diff(f,3)

f3=

-27*cos(3*x)
```

```
>>syms x
>>f=sin(x)
>>int(f)

ans=

-cos(x)
```

```
>>int(f,0,pi)

ans=

2
```

Writing assignment: Exercise 1 @ page 252
Coding assignment: Computer problem 1 @ page 254

Newton-Cotes Formulas for Numerical Integration S1

- Given a function *f* defined on an interval [a, b], two approaches for numerical integration:
- Newton-Cotes approach: Draw an interpolating polynomial through some of the points of $f(x)$ and evaluate the definite integral of the polynomial as the approximation of the integrals.
- Gaussian Quadrature approach: Find a low-degree polynomial approximating the function in the sense of least squares, and evaluate the definite integral of the polynomial as the approximation of the integrals.

Newton-Cotes Formulas for Numerical Integration S2

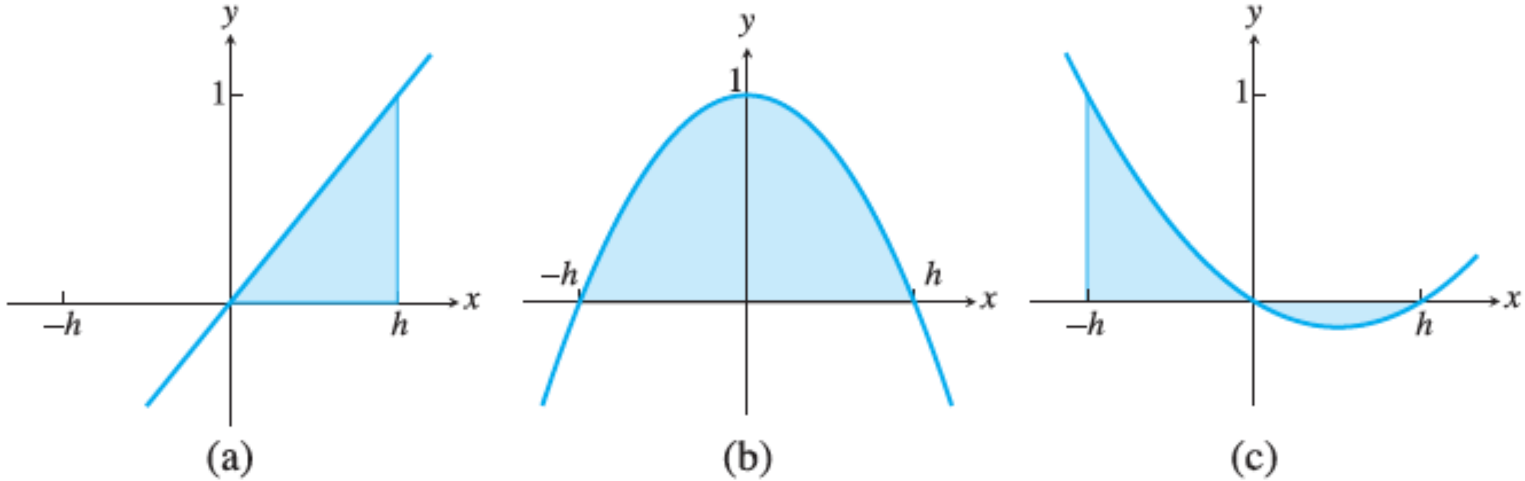


Figure 5.2 Three simple integrals (5.17), (5.18), and (5.19). Net positive area is (a) $h/2$, (b) $4h/3$, and (c) $h/3$.

$(0,0)$ and $(h,1)$

$$\int_0^h \frac{x}{h}\,dx = h/2.$$

$(-h,0)$, $(0,1)$, and $(h,0)$

$$\int_{-h}^{h} P(x)\,dx = x \cancel{- \frac{x^3}{3h^2}} = \frac{4}{3}h.$$

$(-h,0),(0,1),(h,0)$

$$p(x) = 1\frac{(x-(-h))(x-h)}{(0-(-h))(0-h)} = \frac{(x+h)(x-h)}{-h^2}$$

$$\int_{-h}^{h} \frac{(x+h)(x-h)}{-h^2}dx = \frac{1}{-h^2}\int_{-h}^{h} x^2 - h^2\,dx = \frac{2}{-h^2}\left(\frac{1}{3}h^3 - h^3\right) = \frac{4}{3}h$$

$(-h,1)$, $(0,0)$, and $(h,0)$

$$\int_{-h}^{h} P(x)\,dx = \frac{1}{3}h$$

Trapezoid Rule S1

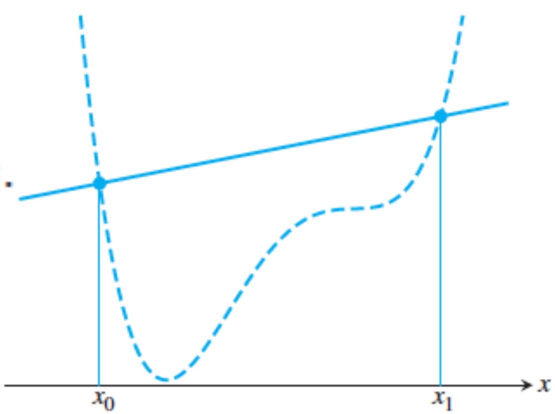
Let $f(x)$ be a function with a continuous second derivative, defined on the interval $[x_0, x_1]$, as shown in Figure 5.3(a). Denote the corresponding function values by $y_0 = f(x_0)$ and $y_1 = f(x_1)$. Consider the degree 1 interpolating polynomial $P_1(x)$ through (x_0, y_0) and (x_1, y_1). Using the Lagrange formulation, we find that the interpolating polynomial with error term is

$$f(x) = y_0 \frac{x - x_1}{x_0 - x_1} + y_1 \frac{x - x_0}{x_1 - x_0} + \frac{(x - x_0)(x - x_1)}{2!} f''(c_x) = P(x) + E(x).$$

It can be proved that the "unknown point" c_x depends continuously on x.

Integrating both sides on the interval of interest $[x_0, x_1]$ yields

$$\int_{x_0}^{x_1} f(x)\, dx = \int_{x_0}^{x_1} P(x)\, dx + \int_{x_0}^{x_1} E(x)\, dx.$$



Trapezoid Rule S2

Computing the first integral gives

$$\begin{aligned}\int_{x_0}^{x_1} P(x)\,dx &= y_0 \int_{x_0}^{x_1} \frac{x - x_1}{x_0 - x_1}\,dx + y_1 \int_{x_0}^{x_1} \frac{x - x_0}{x_1 - x_0}\,dx \\ &= y_0 \frac{h}{2} + y_1 \frac{h}{2} = h \frac{y_0 + y_1}{2}, \end{aligned} \tag{5.20}$$

where we have defined $h = x_1 - x_0$ to be the interval length and computed the integrals by using the fact (5.17). For example, substituting $w = -x + x_1$ into the first integral gives

$$\int_{x_0}^{x_1} \frac{x - x_1}{x_0 - x_1}\,dx = \int_{h}^{0} \frac{-w}{-h}(-dw) = \int_{0}^{h} \frac{w}{h}\,dw = \frac{h}{2},$$

and the second integral, after substituting $w = x - x_0$, is

$$\int_{x_0}^{x_1} \frac{x - x_0}{x_1 - x_0}\,dx = \int_{0}^{h} \frac{w}{h}\,dw = \frac{h}{2}.$$

Formula (5.20) calculates the area of a trapezoid, which gives the rule its name.

Trapezoid Rule S3

The error term is

$$\begin{aligned}\int_{x_0}^{x_1} E(x)\,dx &= \frac{1}{2!}\int_{x_0}^{x_1}(x-x_0)(x-x_1)f''(c(x))\,dx\\ &= \frac{f''(c)}{2}\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx\\ &= \frac{f''(c)}{2}\int_0^h u(u-h)\,du\\ &= -\frac{h^3}{12}f''(c),\end{aligned}$$

where we have used Theorem 0.9, the Mean Value Theorem for Integrals. We have shown:

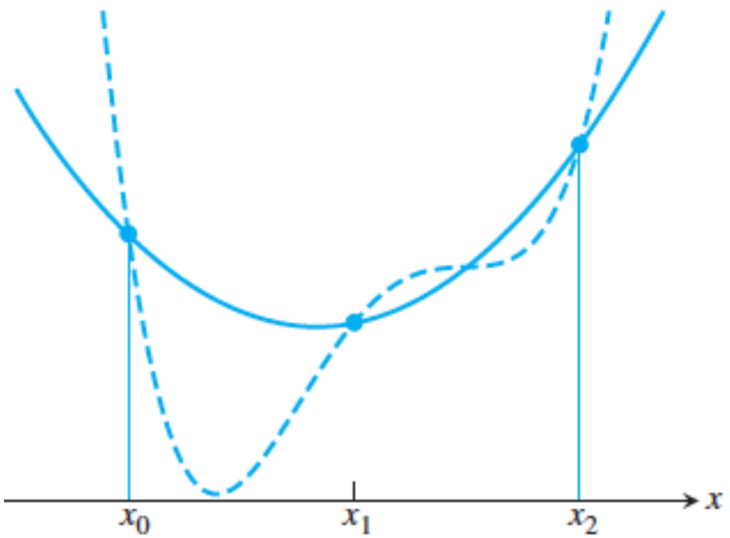
Trapezoid Rule

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}(y_0+y_1) - \frac{h^3}{12}f''(c), \tag{5.21}$$

where $h = x_1 - x_0$ and c is between x_0 and x_1.

Simpson's Rule S1

- Simpson's Rule is similar to the Trapezoid Rule, except that the degree 1 interpolant is replaced by a parabola.



$$
\begin{aligned}
f(x) &= y_0\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + y_1\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \\
&\quad + y_2\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} + \frac{(x-x_0)(x-x_1)(x-x_2)}{3!}f'''(c_x) \\
&= P(x) + E(x).
\end{aligned}
$$

Simpson's Rule S2

Integrating gives

$$\int_{x_0}^{x_2} f(x)\,dx = \int_{x_0}^{x_2} P(x)\,dx + \int_{x_0}^{x_2} E(x)\,dx,$$

where

$$\begin{aligned}\int_{x_0}^{x_2} P(x)\,dx &= y_0 \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)\,dx}{(x_0-x_1)(x_0-x_2)} + y_1 \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)\,dx}{(x_1-x_0)(x_1-x_2)} \\ &\quad + y_2 \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)\,dx}{(x_2-x_0)(x_2-x_1)} \\ &= y_0 \frac{h}{3} + y_1 \frac{4h}{3} + y_2 \frac{h}{3}.\end{aligned}$$

We have set $h = x_2 - x_1 = x_1 - x_0$ and used (5.18) for the middle integral and (5.19) for the first and third.

Simpson's Rule S3

The error term can be computed (proof omitted) as

$$\int_{x_0}^{x_2} E(x)\,dx = -\frac{h^5}{90} f^{(iv)}(c)$$

for some c in the interval $[x_0, x_2]$, provided that $f^{(iv)}$ exists and is continuous. Concluding the derivation yields Simpson's Rule:

Simpson's Rule

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}(y_0 + 4y_1 + y_2) - \frac{h^5}{90} f^{(iv)}(c), \tag{5.22}$$

where $h = x_2 - x_1 = x_1 - x_0$ and c is between x_0 and x_2.

Simpson's Rule S4

- Example

Apply the Trapezoid Rule and Simpson's Rule to approximate

$$\int_1^2 \ln x \, dx,$$

and find an upper bound for the error in your approximations.

The Trapezoid Rule estimates that

$$\int_1^2 \ln x \, dx \approx \frac{h}{2}(y_0 + y_1) = \frac{1}{2}(\ln 1 + \ln 2) = \frac{\ln 2}{2} \approx 0.3466.$$

The error for the Trapezoid Rule is $-h^3 f''(c)/12$, where $1 < c < 2$. Since $f''(x) = -1/x^2$, the magnitude of the error is at most

$$\frac{1^3}{12c^2} \leq \frac{1}{12} \approx 0.0834.$$

Simpson's Rule S5

- Example (cont…)

In other words, the Trapezoid Rule says that

$$\int_1^2 \ln x \, dx = 0.3466 \pm 0.0834.$$

The integral can be computed exactly by using integration by parts:

$$\begin{aligned} \int_1^2 \ln x \, dx &= x \ln x|_1^2 - \int_1^2 dx \\ &= 2\ln 2 - 1\ln 1 - 1 \approx 0.386294. \end{aligned} \tag{5.23}$$

The Trapezoid Rule approximation and error bound are consistent with this result.

Simpson's Rule S6

- Example (cont…)

Simpson's Rule yields the estimate

$$\int_1^2 \ln x\, dx \approx \frac{h}{3}(y_0 + 4y_1 + y_2) = \frac{0.5}{3}\left(\ln 1 + 4\ln\frac{3}{2} + \ln 2\right) \approx 0.3858.$$

The error for Simpson's Rule is $-h^5 f^{(iv)}(c)/90$, where $1 < c < 2$. Since $f^{(iv)}(x) = -6/x^4$, the error is at most

$$\frac{6(0.5)^5}{90c^4} \le \frac{6(0.5)^5}{90} = \frac{1}{480} \approx 0.0021.$$

Thus, Simpson's Rule says that

$$\int_1^2 \ln x\, dx = 0.3858 \pm 0.0021,$$

which is again consistent with the correct value and more accurate than the Trapezoid Rule approximation.

Simpson's Rule S7

- Definition

The **degree of precision** of a numerical integration method is the greatest integer k for which all degree k or less polynomials are integrated exactly by the method. ❒

- The degree of precision of the Trapezoid Rule is 1, since the error term $-h^3 f''(c)/12$ shows that if *f*(x) is a polynomial of degree 1 or less, the error will be zero, and the polynomial will be integrated exactly.
- The degree of precision of the Simpson's Rule is 3, since the error term $-\frac{h^5}{90} f^{(iv)}(c)$ shows that if *f*(x) is a polynomial of degree 3 or less, the error will be zero, and the polynomial will be integrated exactly.

Simpson's Rule S8

- Example

Find the degree of precision of the degree 3 Newton–Cotes formula, called the **Simpson's 3/8 Rule**

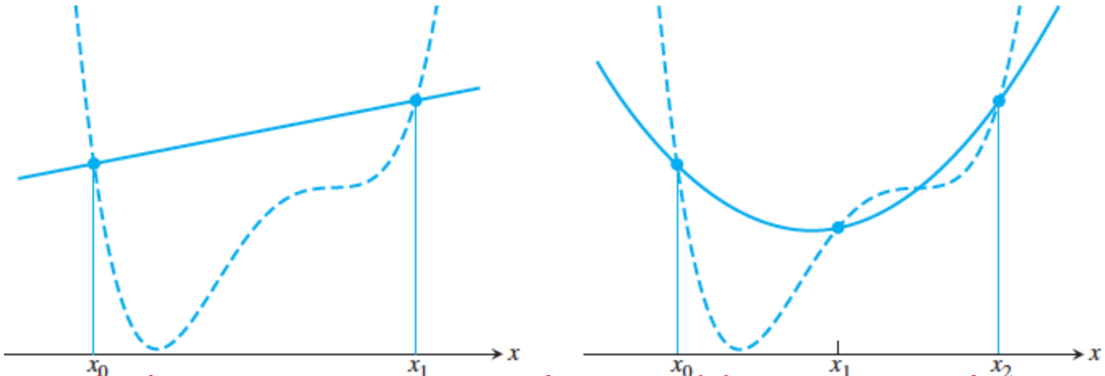
$$\int_{x_0}^{x_3} f(x)dx \approx \frac{3h}{8}(y_0 + 3y_1 + 3y_2 + y_3).$$

It suffices to test monomials in succession. We will leave the details to the reader. For example, when $f(x) = x^2$, we check the identity

$$\frac{3h}{8}(x^2 + 3(x+h)^2 + 3(x+2h)^2 + (x+3h)^2) = \frac{(x+3h)^3 - x^3}{3},$$

the latter being the correct integral of x^2 on $[x, x+3h]$. Equality holds for $1, x, x^2, x^3$, but fails for x^4. Therefore, the degree of precision of the rule is 3. ◀

Composite Newton-Cotes formulas

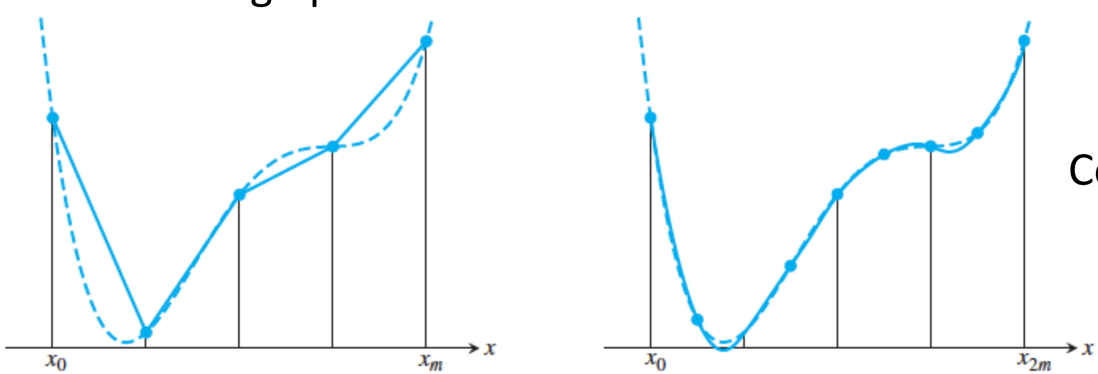


Single numerical integration

Underlying reason: integrals are additive over subintervals

VS

Basic idea: evaluate an integral by dividing the interval up into several subintervals, applying the rule separately on each one, and then totaling up



Composite numerical integration

Composite Trapezoid Rule S1

The composite Trapezoid Rule is simply the sum of Trapezoid Rule approximations on adjacent subintervals, or **panels**.

To approximate

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

consider an evenly spaced grid

$$a = x_0 < x_1 < x_2 < \cdots < x_{m-2} < x_{m-1} < x_m = b$$

along the horizontal axis, where $h = x_{i+1} - x_i$ for each i as shown in Figure 5.4. On each subinterval, we make the approximation with error term

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = \frac{h}{2}(f(x_i) + f(x_{i+1})) - \frac{h^3}{12}f''(c_i),$$

assuming that f'' is continuous.

Composite Trapezoid Rule S2

Adding up over all subintervals (note the overlapping on the interior subintervals) yields

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{m-1} f(x_i)\right] - \sum_{i=0}^{m-1} \frac{h^3}{12} f''(c_i).$$

The error term can be written

$$\frac{h^3}{12}\sum_{i=0}^{m-1} f''(c_i) = \frac{h^3}{12} m f''(c),$$

according to Theorem 5.1, for some $a < c < b$. Since $mh = (b - a)$, the error term is $(b - a)h^2 f''(c)/12$. To summarize, if f'' is continuous on $[a, b]$, then the following holds:

Composite Trapezoid Rule

$$\int_a^b f(x)\,dx = \frac{h}{2}\left(y_0 + y_m + 2\sum_{i=1}^{m-1} y_i\right) - \frac{(b - a)h^2}{12} f''(c) \tag{5.24}$$

where $h = (b - a)/m$ and c is between a and b.

Composite Simpson's Rule S1

The composite Simpson's Rule follows the same strategy. Consider an evenly spaced grid

$$a = x_0 < x_1 < x_2 < \cdots < x_{2m-2} < x_{2m-1} < x_{2m} = b$$

along the horizontal axis, where $h = x_{i+1} - x_i$ for each i. On each length $2h$ panel $[x_{2i}, x_{2i+2}]$, for $i = 0, \ldots, m-1$, a Simpson's Method is carried out. In other words, the integrand $f(x)$ is approximated on each subinterval by the interpolating parabola fit at x_{2i}, x_{2i+1}, and x_{2i+2}, which is integrated and added to the sum. The approximation with error term on the subinterval is

$$\int_{x_{2i}}^{x_{2i+2}} f(x)\,dx = \frac{h}{3}[f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})] - \frac{h^5}{90} f^{(iv)}(c_i).$$

This time, the overlapping is over even-numbered x_j only. Adding up over all subintervals yields

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + f(b) + 4\sum_{i=1}^{m} f(x_{2i-1}) + 2\sum_{i=1}^{m-1} f(x_{2i}) \right] - \sum_{i=0}^{m-1} \frac{h^5}{90} f^{(iv)}(c_i).$$

Composite Simpson's Rule S2

The error term can be written

$$\frac{h^5}{90}\sum_{i=0}^{m-1} f^{(iv)}(c_i) = \frac{h^5}{90} m f^{(iv)}(c),$$

according to Theorem 5.1, for some $a < c < b$. Since $m \cdot 2h = (b-a)$, the error term is $(b-a)h^4 f^{(iv)}(c)/180$. Assuming that $f^{(iv)}$ is continuous on $[a, b]$, the following holds:

Composite Simpson's Rule

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[y_0 + y_{2m} + 4\sum_{i=1}^{m} y_{2i-1} + 2\sum_{i=1}^{m-1} y_{2i}\right] - \frac{(b-a)h^4}{180} f^{(iv)}(c), \quad (5.25)$$

where c is between a and b.

Composite Newton-Cotes formulas

- Example

Carry out four-panel approximations of

$$\int_1^2 \ln x \, dx,$$

using the composite Trapezoid Rule and composite Simpson's Rule.

For the composite Trapezoid Rule on $[1, 2]$, four panels means that $h = 1/4$. The approximation is

$$\begin{aligned}\int_1^2 \ln x \, dx &\approx \frac{1/4}{2}\left[y_0 + y_4 + 2\sum_{i=1}^{3} y_i\right] \\ &= \frac{1}{8}[\ln 1 + \ln 2 + 2(\ln 5/4 + \ln 6/4 + \ln 7/4)] \\ &\approx 0.3837.\end{aligned}$$

The error is at most $\dfrac{(b-a)h^2}{12}|f''(c)| = \dfrac{1/16}{12}\dfrac{1}{c^2} \le \dfrac{1}{(16)(12)(1^2)} = \dfrac{1}{192} \approx 0.0052.$

Composite Newton-Cotes formulas

- Example (cont…)

A four-panel Simpson's Rule sets $h = 1/8$. The approximation is

$$\int_1^2 \ln x \, dx \approx \frac{1/8}{3}\left[y_0 + y_8 + 4\sum_{i=1}^{4} y_{2i-1} + 2\sum_{i=1}^{3} y_{2i}\right]$$

$$= \frac{1}{24}[\ln 1 + \ln 2 + 4(\ln 9/8 + \ln 11/8 + \ln 13/8 + \ln 15/8)$$

$$+ 2(\ln 5/4 + \ln 6/4 + \ln 7/4)]$$

$$\approx 0.386292.$$

This agrees within five decimal places with the correct value 0.386294 from (5.23). Indeed, the error cannot be more than

$$\frac{(b-a)h^4}{180}|f^{(iv)}(c)| = \frac{(1/8)^4}{180}\frac{6}{c^4} \le \frac{6}{8^4 \cdot 180 \cdot 1^4} \approx 0.000008.$$

Composite Newton-Cotes formulas

- Example

Find the number of panels m necessary for the composite Simpson's Rule to approximate

$$\int_0^{\pi} \sin^2 x \, dx$$

within six correct decimal places.

We require the error to satisfy

$$\frac{(\pi - 0)h^4}{180} |f^{(iv)}(c)| < 0.5 \times 10^{-6}.$$

Since the fourth derivative of $\sin^2 x$ is $-8\cos 2x$, we need

$$\frac{\pi h^4}{180} 8 < 0.5 \times 10^{-6},$$

or $h < 0.0435$. Therefore, $m = \texttt{ceil}(\pi/(2h)) = 37$ panels will be sufficient. ◀

Open Newton-Cotes Methods S1

- Closed Newton-Cotes Methods: Trapezoid Rule and Simpson's Rule Both use interval endpoints, i.e., require input values from the ends of the integration interval.
- Open Newton-Cotes Methods: which does not use values from the endpoints, especially useful for the integrands that have a removable singularity at an interval endpoint

Open Newton-Cotes Methods S2

Midpoint Rule

$$\int_{x_0}^{x_1} f(x)\,dx = hf(w) + \frac{h^3}{24} f''(c), \tag{5.26}$$

where $h = (x_1 - x_0)$, w is the midpoint $x_0 + h/2$, and c is between x_0 and x_1.

- The Midpoint Rule is also useful for cutting the number of function evaluations needed.
- Compared with the Trapezoid Rule, the closed Newton–Cotes Method of the same order, it requires one function evaluation rather than two.
- The error term is half the size of the Trapezoid Rule error term.

Open Newton-Cotes Methods S3

The proof of (5.26) follows the same lines as the derivation of the Trapezoid Rule. Set $h = x_1 - x_0$. The degree 1 Taylor expansion of $f(x)$ about the midpoint $w = x_0 + h/2$ of the interval is

$$f(x) = f(w) + (x - w)f'(w) + \frac{1}{2}(x - w)^2 f''(c_x),$$

where c_x depends on x and lies between x_0 and x_1. Integrating both sides yields

$$\begin{aligned}
\int_{x_0}^{x_1} f(x)\,dx &= (x_1 - x_0)f(w) + f'(w)\int_{x_0}^{x_1}(x - w)\,dx + \frac{1}{2}\int_{x_0}^{x_1} f''(c_x)(x - w)^2\,dx \\
&= hf(w) + 0 + \frac{f''(c)}{2}\int_{x_0}^{x_1}(x - w)^2\,dx \\
&= hf(w) + \frac{h^3}{24}f''(c),
\end{aligned}$$

where $x_0 < c < x_1$. Again, we have used the Mean Value Theorem for Integrals to pull the second derivative outside of the integral. This completes the derivation of (5.26).

Open Newton-Cotes Methods S4

Composite Midpoint Rule

$$\int_a^b f(x)\,dx = h\sum_{i=1}^{m} f(w_i) + \frac{(b-a)h^2}{24} f''(c), \qquad (5.27)$$

where $h = (b-a)/m$ and c is between a and b. The w_i are the midpoints of the m equal subintervals of $[a, b]$.

Another useful open Newton–Cotes Rule is

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{4h}{3}[2f(x_1) - f(x_2) + 2f(x_3)] + \frac{14h^5}{45} f^{(iv)}(c), \qquad (5.28)$$

where $h = (x_4 - x_0)/4, x_1 = x_0 + h, x_2 = x_0 + 2h, x_3 = x_0 + 3h$, and where $x_0 < c < x_4$.

Open Newton-Cotes Methods S5

- Example

Approximate $\int_0^1 \sin x/x \, dx$ by using the Composite Midpoint Rule with $m = 10$ panels.

First note that we cannot apply a closed method directly to the problem, without special handling at $x = 0$. The midpoint method can be applied directly. The midpoints are $0.05, 0.15, \ldots, 0.95$, so the Composite Midpoint Rule delivers

$$\int_0^1 f(x)\, dx \approx 0.1 \sum_1^{10} f(m_i) = 0.94620858.$$

The correct answer to eight places is 0.94608307.

Writing assignment: Exercise 1 @ page 263
Coding assignment: Computer problem 1 @ page 264