Numerical Differentiation and Integration

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Overview

- Numerical Differentiation
- Richardson's Extrapolation
- Numerical Integration
  - Elements of Numerical Integration
  - Composite of Numerical Integration
  - Romberg Integration
  - Adaptive Quadrature Methods

Numerical Differentiation

Problem. Given

$$f: \mathbb{R} \longrightarrow \mathbb{R},$$

$$x_0, x_1, \ldots, x_n, \quad x_i \in \mathbb{R},$$

compute

$$f'(x_i), \quad i = 0, 1, \ldots, n.$$

Main tool. Lagrange interpolating polynomials.

Issues to look at. Approximation, truncation error, effect of round-off error.

Lagrange Interpolating Polynomials - a Review

Theorem 1

$$\left.\begin{array}{l} f \in C^{n+1}[a,b] \\ x_0, x_1, \ldots, x_n,\ x_i \in [a,b] \\ x_i \neq x_j \text{ for } i \neq j \end{array}\right\} \Longrightarrow \begin{array}{c} \forall\, x \in [a,b],\ \exists\, \xi(x) \in (a,b)\ s.t. \\ f(x) = P(x) + R(x) \end{array}$$

where $P(x)$ is the Lagrange interpolating polynomial

$$P(x) = \sum_{k=0}^{n} f(x_k) L_k(x) = f(x_0)L_0(x) + \cdots + f(x_n)L_n(x),$$

and $R(x)$ is the remainder term

$$R(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)(x-x_1)\cdots(x-x_n).$$

Numerical Differentiation – Main Idea

$$
\left.\begin{array}{cccc}
x_0 & x_1 & \dots & x_n \\
\downarrow & \downarrow & & \downarrow \\
f(x_0) & f(x_1) & \dots & f(x_n)
\end{array}\right\} \Longrightarrow \left\{\begin{array}{l}
f(x) = P(x) + R(x) \\
f'(x) = P'(x) + R'(x) \\
f'(x_i) = P'(x_i) + R'(x_i)
\end{array}\right.
$$

A special case. The nodes $x_0, x_1, \dots, x_n$ are equally spaced, i.e.,

$$x_1 = x_0 + h,\ x_2 = x_0 + 2h, \dots, x_i = x_0 + ih, \dots, x_n = x_0 + nh.$$

Numerical Differentiation – $(n+1)$-Point Formula

Since

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x)),$$

$$\begin{aligned} f'(x) &= \sum_{k=0}^{n} f(x_k)L_k'(x) + D_x\left(\frac{(x-x_0)\cdots(x-x_n)}{(n+1)!}\right) f^{(n+1)}(\xi(x)) \\ &\quad + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} D_x(f^{(n+1)}(\xi(x))). \end{aligned}$$

Hence, for $0 \le j \le n$,

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L_k'(x_j) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{k=0, k\neq j}^{n} (x_j - x_k) \qquad (1)$$

2-Point Formula

For x_0, $x_1 = x_0 + h$, it follow from (1) that

$$\begin{aligned} f'(x_0) &= f(x_0)L_0'(x_0) + f(x_1)L_1'(x_0) + \frac{f''(\xi(x))}{2}(x_0 - x_1) \\ &= f(x_0)\frac{1}{x_0 - x_1} + f(x_1)\frac{1}{x_1 - x_0} - \frac{h}{2}f''(\xi(x)) \\ &= \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2}f''(\xi). \end{aligned} \tag{2}$$

If $h > 0 \Longrightarrow$ **forward-difference formula.**

If $h < 0 \Longrightarrow$ **backward-difference formula.**

2-Point Formula – an Example

Let $f(x) = \ln(x)$, and $x_0 = 1.8$. The forward-difference formula

$$\frac{f(1.8+h) - f(1.8)}{h}$$

is used to approximate $f'(1.8)$ with error

$$\frac{|hf''(\xi)|}{2} = \frac{|h|}{2\xi^2} \leq \frac{|h|}{2(1.8)^2}, \quad \text{where } 1.8 < \xi < 1.8 + h.$$

3-Point Formula

For given x_0, x_1, x_2, it follow from (1) that

$$
\begin{aligned}
f'(x_j) &= f(x_0)\left(\frac{2x_j - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}\right) + f(x_1)\left(\frac{2x_j - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}\right) + \\
&\quad f(x_2)\left(\frac{2x_j - x_0 - x_1}{(x_2-x_0)(x_2-x_1)}\right) + \frac{1}{6} f^{(3)}(\xi_j) \prod_{k=0, k\neq j}^{2} (x_j - x_k), \quad (3)
\end{aligned}
$$

for each $j = 0, 1, 2$, where ξ_j indicates this point depends on x_j.

Equally-spaced nodes. For ξ_0 between x_0 and $x_0 + 2h$, and ξ_1 between $x_0 - h$ and $x_0 + h$:

$$
\begin{aligned}
f'(x_0) &= \frac{1}{2h}\left(-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right) + \frac{h^2}{3} f^{(3)}(\xi_0), \quad (4) \\
f'(x_0) &= \frac{1}{2h}\left(f(x_0+h) - f(x_0-h)\right) - \frac{h^2}{6} f^{(3)}(\xi_1). \quad (5)
\end{aligned}
$$

3-Point Formula – an Example

Use the most appropriate three point formula to determine approximations that complete the following table:

x	$f(x)$	$f'(x)$
1.1	9.025013	17.769705
1.2	11.02318	22.193635
1.3	13.46374	27.107350
1.4	16.44465	32.510850

$$
\begin{aligned}
f'(1.1) &\overset{(4)}{\approx} \tfrac{1}{2(0.1)}(-3f(1.1)+4f(1.2)-f(1.3)) &= 17.769705 \\
f'(1.2) &\overset{(5)}{\approx} \tfrac{1}{2(0.1)}(f(1.3)-f(1.1)) &= 22.193635 \\
f'(1.3) &\overset{(5)}{\approx} \tfrac{1}{2(0.1)}(f(1.4)-f(1.2)) &= 27.107350 \\
f'(1.4) &\overset{(4)}{\approx} \tfrac{1}{2(-0.1)}(-3f(1.4)+4f(1.3)-f(1.2)) &= 32.510850
\end{aligned}
$$

3-Point Formula – Remarks

- At the end points, we must use one sided differences.
- In the interior, we use centered differences. They have a smaller error constant when f is smooth and require fewer operations to compute.

5-Point Formula

Centered differences. For ξ between $x_0 - 2h$ and $x_0 + 2h$:

$$f'(x_0) = \frac{1}{120}\left(f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)\right) + \frac{h^4}{30} f^{(5)}(\xi). \tag{6}$$

One-sided differences. For ξ between x_0 and $x_0 + 4h$:

$$f'(x_0) = \frac{1}{120}\left(-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) 16f(x_0 + 3h) - 3f(x_0 + 4h)\right) + \frac{h^4}{5} f^{(5)}(\xi). \tag{7}$$

Higher-Order Derivatives

Consider finding the second derivative of f:

1. expand f in a third Taylor polynomial about a point x_0, and
2. evaluate at $x_0 + h$ and $x_0 - h$:

$$
\begin{aligned}
f(x_0+h) &= f(x_0)+f'(x_0)h+\frac{1}{2}f''(x_0)h^2+\frac{1}{6}f'''(x_0)h^3+\frac{1}{24}f^{(4)}(\xi_1)h^4 \quad (8) \\
f(x_0-h) &= f(x_0)-f'(x_0)h+\frac{1}{2}f''(x_0)h^2-\frac{1}{6}f'''(x_0)h^3+\frac{1}{24}f^{(4)}(\xi_{-1})h^4 \quad (9)
\end{aligned}
$$

where $x_0 - h < \xi_{-1} < x_0 < \xi_1 < x_0 + h$.

$$
\stackrel{(8)+(9)}{\Longrightarrow} f(x_0+h) + f(x_0-h) = 2f(x_0)+f''(x_0)h^2+\frac{1}{24}(f^4(\xi_1)+f^{(4)}(\xi_{-1}))h^4
$$

Hence,

$$
\begin{aligned}
f''(x_0) \quad = \quad & \frac{1}{h^2}\left(f(x_0-h)-2f(x_0)+f(x_0+h)\right)- \\
& \frac{h^2}{24}\left(f^{(4)}(\xi_1)+f^{(4)}(\xi_{-1})\right). \qquad (10)
\end{aligned}
$$

$$
\left.\begin{array}{l}
\bullet \text{ Suppose } f^{(4)} \in C[x_0-h, x_0+h] \\
\bullet\ K = \frac{1}{2}\left(f^{(4)}(\xi_1)+f^{(4)}(\xi_{-1})\right) \\
\quad \text{between } f^{(4)}(\xi_1) \text{ and } f^{(4)}(\xi_{-1})
\end{array}\right\} \overset{\text{IVT}}{\Longrightarrow} \begin{array}{l} \exists \xi \in (\xi_{-1}, \xi_1) \\ \quad \text{s.t. } f^{(4)}(\xi) = K. \end{array}
$$

By (10),

$$
f''(x_0) = \frac{1}{h^2}\left(f(x_0-h)-2f(x_0)+f(x_0+h)\right) - \frac{h^2}{12} f^{(4)}(\xi), \qquad (11)
$$

for some ξ, where $x_0 - h < \xi < x_0 + h$.

Effect of Round-Off Error

Consider the centered-difference 3-point formula (5):

$$f'(x_0) = \frac{1}{2h}\left(f(x_0+h) - f(x_0-h)\right) - \frac{h^2}{6} f^{(3)}(\xi_1).$$

Let

$$\begin{aligned} f(x_0+h) &= \tilde{f}(x_0+h) + e(x_0+h) \\ f(x_0-h) &= \tilde{f}(x_0-h) + e(x_0-h). \end{aligned}$$

Then

$$f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} = \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1).$$

If

$$\left.\begin{array}{l} |e(x_0 \pm h)| \leq \epsilon \\ |f^{(3)}| \leq M \end{array}\right\} \Longrightarrow Err_{abs} \leq \frac{\epsilon}{h} + \frac{h^2}{6}M.$$

$$\left(\frac{h^2}{6}M\right) \searrow \ \Longrightarrow \left(\frac{\epsilon}{h}\right) \nearrow .$$

To reduce the truncation error, $h^2M/6$, we must reduce h. However, as h is reduced, the roundoff error ϵ/h grows. In practice, it is seldom advantageous to let h be too small since the roundoff error will dominate the calculations.

Remark 1 Similar difficulties occur with all differentiation formulas, and numerical differentiation is *unstable*.

Richardson's Extrapolation

Suppose

$$\underbrace{M}_{\text{exact}} - \underbrace{N_1(h)}_{\text{computed}} = \underbrace{K_1 h + K_2 h^2 + K_3 h^3 + \cdots}_{\text{truncation error}}, \quad K_i \in \mathbb{R}. \qquad (12)$$

Remark 2 The truncation error is dominated by $K_1 h$ when h is small $\longrightarrow O(h)$ approximation.

Goal. Obtain higher order approximations, e.g., $O(h^2)$, $O(h^3), \ldots$

$\mathbf{O(h^2)}$ Approximation

$$
\begin{aligned}
M &\overset{(12)}{=} N_1\left(\frac{h}{2}\right) + K_1\left(\frac{h}{2}\right) + K_2\left(\frac{h}{2}\right)^2 + K_3\left(\frac{h}{2}\right)^3 + \cdots && (13)\\
&\overset{2(13)-(12)}{=} \underbrace{\left(N_1\left(\frac{h}{2}\right) + \left(N_1\left(\frac{h}{2}\right) - N(h)\right)\right)}_{N_2(h)} + \\
&\quad K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots && (14)
\end{aligned}
$$

Hence,

$$
M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots .
$$

Note. To compute $N_2(h)$, one needs $N_1(h)$ and $N_1(h/2)$.

$\mathbf{O(h^3), O(h^4), O(h^5)}$ Approximations

To obtain higher-order approximations, repeat the same process.

$O(h^3)$: Set

$$N_3 = N_2\left(\frac{h}{2}\right) + \frac{N_2(h/2) - N_2(h)}{2^2 - 1}.$$

Then

$$M = N_3(h) + \frac{K_3}{8}h^3 + \cdots$$

$O(h^4)$:

$$N_4 = N_3\left(\frac{h}{2}\right) + \frac{N_3(h/2) - N_3(h)}{2^3 - 1}.$$

$O(h^5)$:

$$N_5 = N_4\left(\frac{h}{2}\right) + \frac{N_4(h/2) - N_4(h)}{2^4 - 1}.$$

$\mathbf{O(h^j)}$ Approximation

In general, if M can be written in the form

$$
\begin{aligned}
M &= N_1(h) + \sum_{j=1}^{m-1} K_j h^j + O(h^m) \\
&= N_1(h) + K_1 h + K_2 h^2 + \cdots + K_{m-1} h^{m-1} + O(h^m),
\end{aligned}
$$

then for each $j = 2, 3, \ldots, m$, we have an $O(h^j)$ approximation of the form

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{2^{j-1} - 1}.$$

Remark 3 Higher order approximations can be *systematically* derived from lower order approximations:

$$
\begin{array}{cccc}
O(h) & O(h^2) & O(h^3) & O(h^4) \\
N_1(h) & & & \\
N_1(h/2) & N_2(h) & & \\
N_1(h/4) & N_2(h/2) & N_3(h) & \\
N_1(h/8) & N_2(h/4) & N_3(h/2) & N_4(h)
\end{array}
$$

Remark 4 Extrapolation can be applied whenever the truncation error for a formulas has the form

$$\sum_{j=1}^{m-1} K_j h^{\alpha_j} + O(h^{\alpha_m}),$$

for $K_j \in \mathbb{R}$ and $\alpha_1 < \alpha_2 < \cdots < \alpha_m$.

Richardson's Extrapolation – an Example

The centered difference formula to approximate $f'(x_0)$:

$$f'(x_0) = \underbrace{\frac{1}{2h}\left(f(x_0+h) - f(x_0-h)\right)}_{N_1(h)} - \underbrace{\frac{f^{(3)}(x_0)}{6}}_{K_2} h^2 - \underbrace{\frac{f^{(5)}(x_0)}{120}}_{K^4} h^4 - \cdots \tag{15}$$

$$\stackrel{(15)}{\Longrightarrow} f'(x_0) = N_1\left(\frac{h}{2}\right) - \frac{h^2}{24} f^{(3)}(x_0) - \frac{h^4}{1920} f^{(5)}(x_0) - \cdots \tag{16}$$

$$\stackrel{4(16)-(15)}{\Longrightarrow} f'(x_0) = \underbrace{N_1\left(\frac{h}{2}\right) + \frac{N_1(h/2) - N_1(h)}{3}}_{N_2(h)} + \frac{h^4}{160} f^{(5)}(x_0) + \cdots \tag{17}$$

Continuing this procedure gives, for each $i = 2, 3, \ldots$, an $O(h^{2j})$ approximation

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1}.$$

Suppose $x_0 = 2.0, h = 0.2$, and $f(x) = xe^x$. Then

$$\begin{aligned} N_1(0.2) &= \frac{1}{0.4}(f(2.2) - f(1.8)) = 22.414160 \\ N_1(0.1) &= 22.228786 \\ N_1(0.05) &= 22.182564 \end{aligned}$$

$N_1(0.2)$		
$N_1(0.1)$	$N_2(0.2) = N_1(0.1) +$ $(N_1(0.1) - N_1(0.2))/3$	
$N_1(0.05)$	$N_2(0.1) = N_1(0.005) +$ $(N_1(0.05) - N_1(0.1))/3$	$N_3(0.2) = N_2(0.1) + \frac{N_2(0.1) - N_2(0.2)}{15}$

Remark 5 Extrapolation can produce high order approximations with minimal computational cost.

Remark 6 It is important to be aware that as higher order extrapolations are used, more roundoff error will be generated. We may also increase the likelihood of numerical instabilities in some situations.

Numerical Integration

To compute

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

write

$$f(x) = P_n(x) + R_n(x), \quad P_n(x) \in \mathbb{R}[x].$$

Hence,

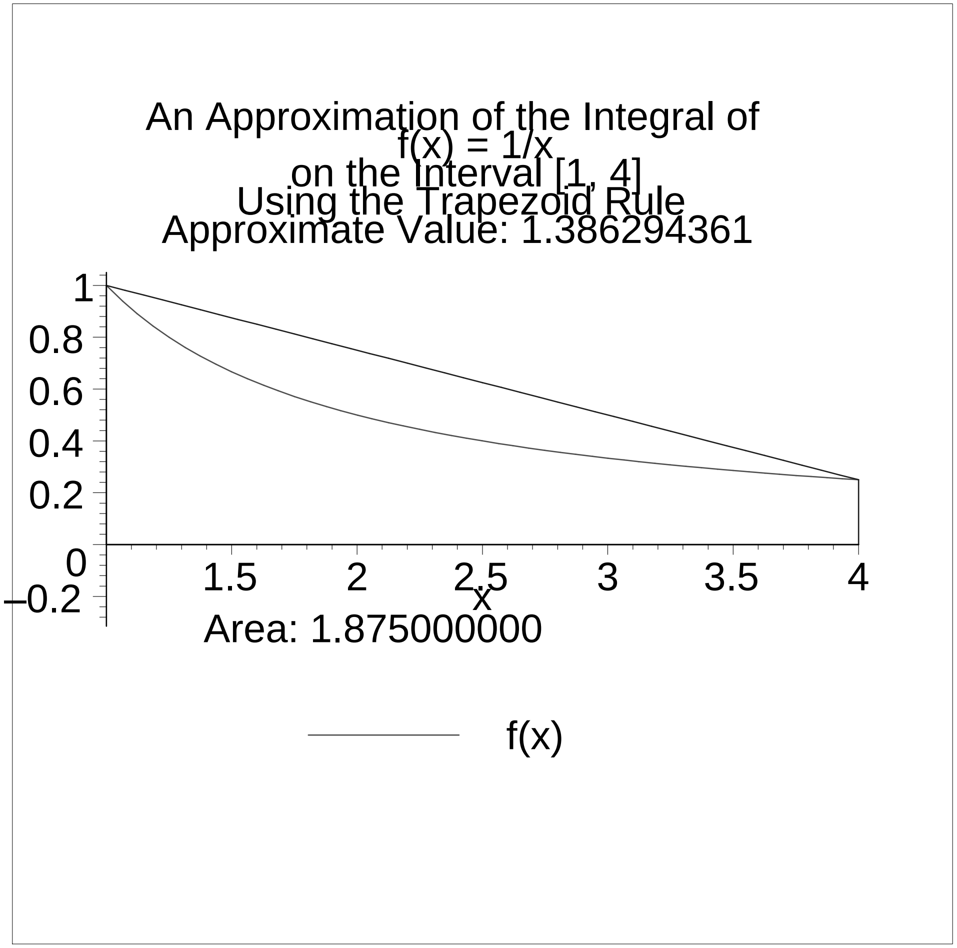
$$I_e = \underbrace{\int_a^b P_n\,(x)\,dx}_{I_a} + \underbrace{\int_a^b R_n\,(x)\,dx}_{E}\,.$$

Main Tools.

(a) polynomial interpolation, Taylor's theorem,

(b) piecewise approach + (a).

Trapezoidal Rule



Let

$$x_0 = a, \quad x_1 = b, \quad h = b - a.$$

Then

$$f(x) = P_1(x) + R_1(x),$$

where

$$\begin{aligned} P_1(x) &= \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1), \\ R_1(x) &= f''(\xi(x))(x - x_0)(x - x_1). \end{aligned}$$

Hence,

$$I_e = \int_a^b f(x)\, dx = \frac{h}{2}(f(x_0) + f(x_1)) + \int_a^b R_1(x) dx.$$

To approximate the error E, we need the

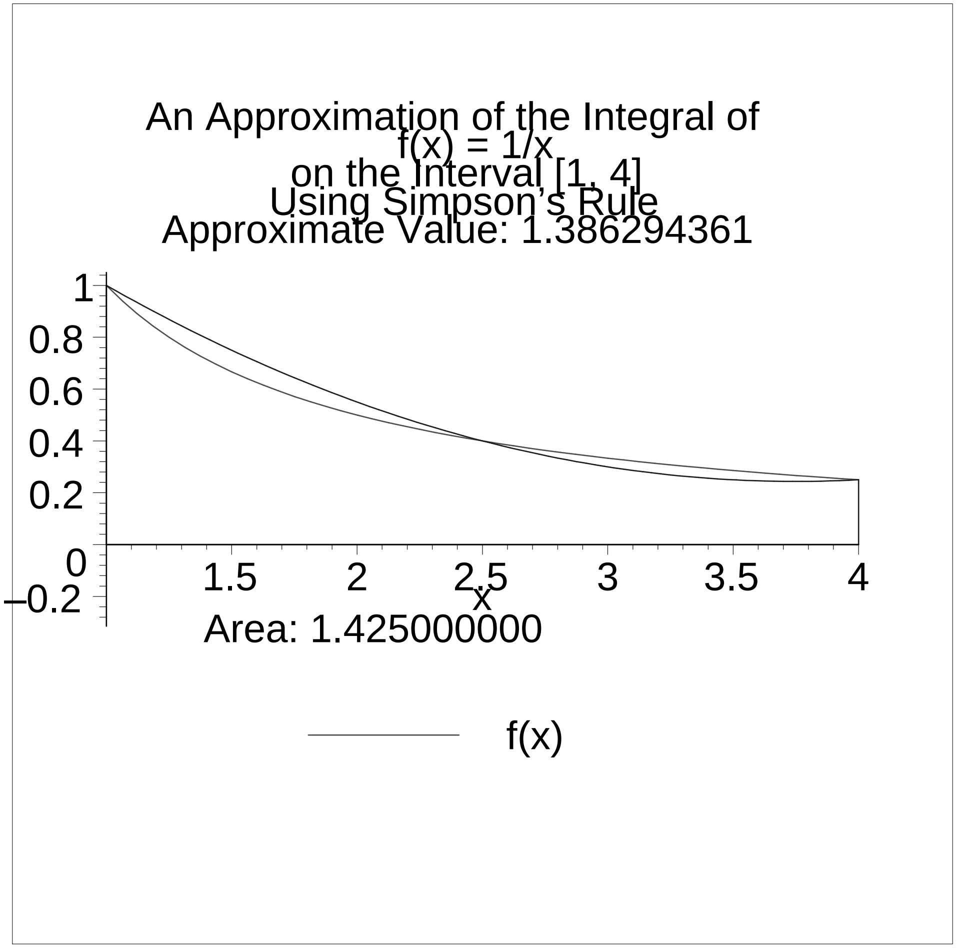
Theorem 2 *Weighted Mean Value Theorem for integrals.*

$$\left.\begin{array}{l} h \in C[a,b] \\ \textit{Riemann integral of } g \textit{ exists} \\ g(x) \textit{ does not change sign on } [a,b] \end{array}\right\} \Longrightarrow \begin{array}{l} \exists c \in (a,b) \textit{ with} \\ \int_a^b h(x)g(x)dx = \\ \quad h(c) \int_a^b g(x)dx. \end{array}$$

$$\begin{aligned} E &= \frac{1}{2}\int_{x_0}^{x_1} \underbrace{f''(\xi(x))}_{h}\underbrace{(x-x_0)(x-x_1)}_{g}\,dx \\ &\overset{WMVT}{=} \frac{1}{2} f''(\xi)\int_{x_0}^{x_1}(x-x_0)(x-x_1)dx, \quad \xi \in (x_0, x_1) \\ &= -\frac{h^3}{12} f''(\xi). \end{aligned}$$

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

Simpson's Rule



Let $x_0 = a, \;\; x_1 = a+h, \;\; x_2 = b, \quad$ where $\; h = \dfrac{b-a}{2}.$

By Taylor's theorem,

$$\begin{aligned}
f(x) &= P_3(x) + R_3(x), \quad \text{where} \\
P_3(x) &= f(x_1) + f'(x_1)(x-x_1) + \\
&\quad \frac{f''(x_1)}{2}(x-x_1)^2 + \frac{f'''(x_1)}{6}(x-x_1)^3, \\
R_3(x) &= \frac{f^{(4)}(\xi(x))}{24}(x-x_1)^4.
\end{aligned}$$

Hence,

$$\int_{x_0}^{x_2} f(x)dx = 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \underbrace{\int_{x_0}^{x_2} \frac{f^{(4)}(\xi(x))}{24}(x-x_1)^4 dx}_{E_1}. \tag{18}$$

$$
\begin{aligned}
E_1 &\overset{WMVT}{=} \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x-x_1)^4dx, \;\; \xi_1 \in (a,b) \\
&= \frac{f^{(4)}(\xi_1)}{60}h^5.
\end{aligned} \tag{19}
$$

By (11),

$$
f''(x_1) = \frac{1}{h^2}(f(x_0) - 2f(x_1) + f(x_2)) + \frac{h^2}{12}f^{(4)}(\xi_2). \tag{20}
$$

By (18), (19), and (20),

$$
\begin{aligned}
\int_{x_0}^{x_2} f(x)dx &= \frac{h}{3}(f(x_0){+}4f(x_1){+}f(x_2)){-}\frac{h^5}{12}(\frac{1}{3}f^{(4)}(\xi_2){-}\frac{1}{5}f^{(4)}(\xi_1)) \\
&= \frac{h}{3}(f(x_0){+}4f(x_1){+}f(x_2)){-}\frac{h^5}{90}f^{(4)}(\xi), \; \xi \in (x_0, x_2).
\end{aligned}
$$

Degree of Accuracy

Definition 1 *The* degree of accuracy, *or* precision, *of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \ldots, n$.*

Remark 7 The Trapezoidal and Simpson's rules have degrees of precision one and three, respectively.

Closed Newton-Cotes Formulas

Let

$$x_0 = a,\ x_n = b,\ h = \frac{b-a}{n},\ x_i = x_0 + ih,\ 0 \le i \le n.$$

Then

$$\begin{aligned}
\int_a^b f(x)dx &\approx \int_a^b \sum_{i=0}^{n} L_i(x) f(x_i) \\
&= \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)dx \\
&= \sum_{i=0}^{n} a_i f(x_i), \quad a_i = \int_a^b L_i(x)dx.
\end{aligned}$$

The formula is *closed* because the endpoints of the interval are included as nodes.

Error Analysis

Theorem 3 *Suppose that*

$$\sum_{i=0}^{n} a_i f(x_i)$$

denotes the $(n+1)$*-point closed Newton-Cotes formula with*

$$x_0 = a, \quad x_n = b, \quad \text{and} \quad h = \frac{b-a}{n}.$$

There exists $\xi \in (a,b)$ *for which*

$$\begin{aligned} \int_a^b f(x)dx &= \sum_{i=0}^{n} a_i f(x_i) + \\ & \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)dt, \end{aligned}$$

if n *is even and* $f \in C^{n+2}[a,b]$*, and*

$$
\begin{aligned}
\int_a^b f(x)dx &= \sum_{i=0}^{n} a_i f(x_i) + \\
&\quad \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)dt,
\end{aligned}
$$

if n is odd and $f \in C^{n+1}[a,b]$.

Remark 8 If n is even, the degree of precision if $n+1$, and the error is $O(h^{n+3})$.

If n is odd, the degree of precision if n, and the error is $O(h^{n+2})$.

Some Common Cases

$n = 1$: Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f(x_0) + f(x_1)) - \frac{h^3}{12} f''(\xi), \;\; x_0 < \xi < x_1.$$

$n = 2$: Simpson's rule

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) - \frac{h^5}{90} f^{(4)}(\xi), \;\; x_0 < \xi < x_2.$$

$n = 3$: Simpson's Three-Eighth rule

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

where $x_0 < \xi < x_3$.

Open Newton-Cotes Formulas

For open Newton-Cotes formulas,

$$x_i = x_0 + ih,\ 0 \le i \le n,\ \ x_0 = a + h,\ h = \frac{b-a}{n+2},$$

and

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

Note that $x_0 = a + h$ and $x_n = b - h$. The formulas are *open* because the nodes are all contained in the open interval (a, b).

Error analysis. If n is even, the degree of precision is $n+1$ and the error is $O(h^{n+3})$.

If n is odd, the degree of precision is only n and the error is only $O(h^{n+2})$.

Some common cases.

$n = 0$: Midpoint rule

$$\int_a^b f(x)dx = 2hf(x_0) + \frac{h^3}{3} f''(\xi), \quad \xi \in (a,b).$$

$n = 1$:

$$\int_a^b f(x)dx = \frac{3h}{2}(f(x_0) + f(x_1)) + \frac{3h^3}{4} f''(\xi), \quad \xi \in (a,b).$$

$n = 2$:

$$\int_a^b f(x)dx = \frac{4h}{3}(2f(x_0) - f(x_1) + 2f(x_2)) + \frac{14h^5}{45} f^{(4)}(\xi), \quad \xi \in (a,b).$$

Composite Numerical Integration

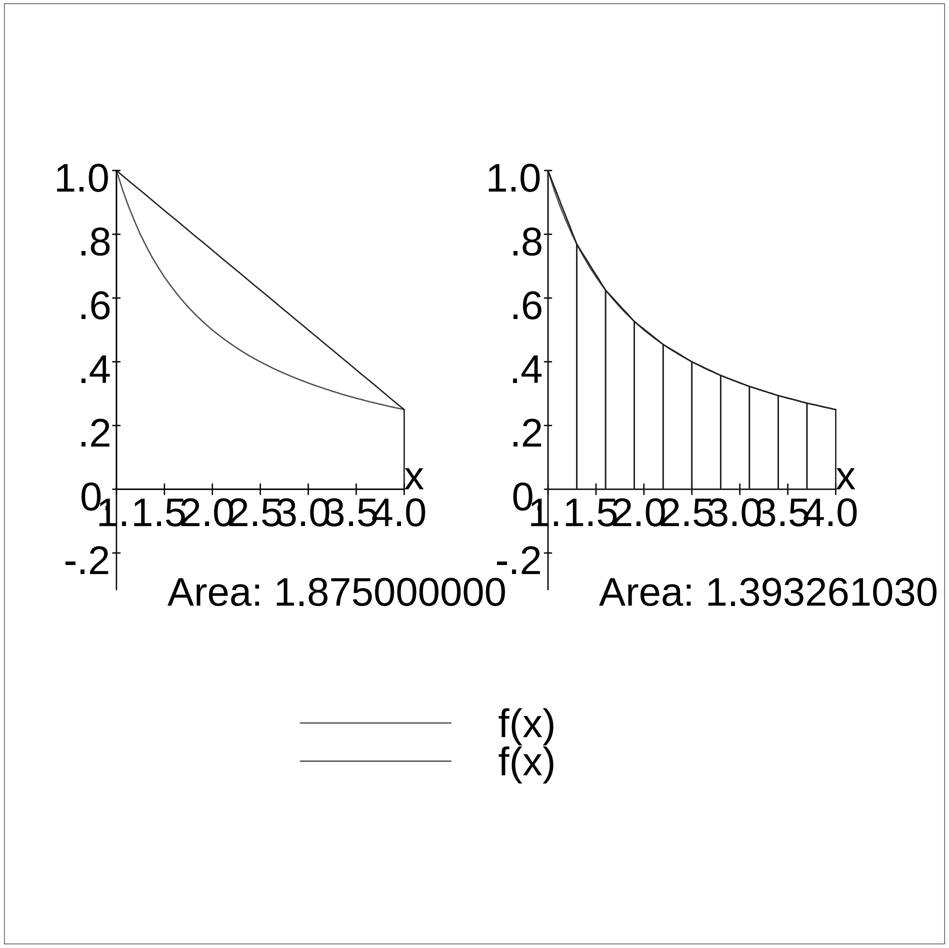
Typically, we do not apply Newton-Cotes formulas to the interval $[a, b]$ directly.

If we did, then high degree formulas would be required to obtain accurate solutions.

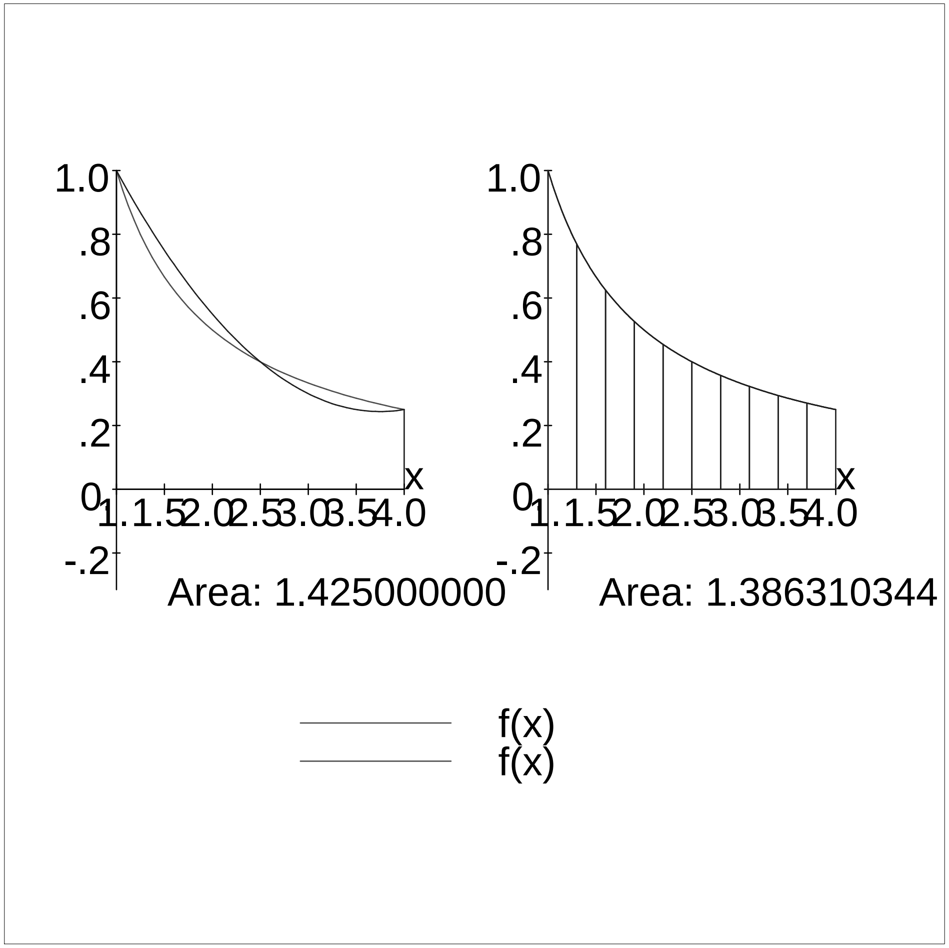
However, we have already seen that even these high degree polynomials often give an oscillatory (and inaccurate) interpolation of high degree polynomials.

To avoid this problem, we prefer a *piecewise approach to numerical integration that uses low order Newton-Cotes formulas.*

Composite Trapezoidal – an Illustration



Composite Simpson – an Illustration



Composite Simpson's Rule

Divide the interval into an *even* number of subintervals, and apply Simpson's rule on each consecutive pair of subintervals.

Take $h = (b-a)/n$, $x_j = a + jh$. Then

$$\begin{aligned}
\int_a^b f(x)dx &= \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)dx \\
&= \sum_{j=1}^{n/2} \left(\frac{h}{3} \left(f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})\right) - \frac{h^5}{90} f^{(4)}(\xi_j) \right) \\
&= \frac{h}{3}\left(f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\right) + E,
\end{aligned}$$

where $E = -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j)$, $x_{2j-2} < \xi_j < x_{2j}$, and $f \in C^4[a,b]$.

To simplify E, we need the

Theorem 4 *Extreme Value Theorem (EVT)*

If $h \in C[a,b]$, then $C_1, C_2 \in [a,b]$ exists with

$$h(C_1) \le h(x) \le h(C_2) \quad \textit{for each} \;\; x \in [a,b].$$

If $f \in C^4[a,b]$, then by the EVT

$$\min_{x\in[a,b]} f^{(4)}(x) \le f^{(4)}(\xi_j) \le \max_{x\in[a,b]} f^{(4)}(x).$$

Sum over all j:

$$\frac{n}{2}\min_{x\in[a,b]} f^{(4)}(x) \le \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \frac{n}{2}\max_{x\in[a,b]} f^{(4)}(x).$$

Multiply by $2/n$:

$$\min_{x\in[a,b]} f^{(4)}(x) \leq \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j) \leq \max_{x\in[a,b]} f^{(4)}(x).$$

By the IVT, there is a $\mu \in (a,b)$ s.t.

$$f^{(4)}(\mu) = \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

Hence,

$$\begin{aligned} E &= -\frac{hn}{180}h^4 f^{(4)}(\mu) \\ &= -\frac{b-a}{180}h^4 f^{(4)}(\mu). \end{aligned}$$

Remark 9 The subdivision approach can be applied to any of the low order formulas. For example:

Theorem 5 *Let* $f \in C^2[a,b]$,

$$h = \frac{b-a}{n}, \quad \textit{and} \;\; x_j = a + jh, \quad \textit{for each } j = 0, 1, \ldots, n.$$

There exists a $\mu \in (a,b)$ *for which the* composite trapezoidal rule *for* n *subintervals can be written with its error term as*

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

An Example

Show that the error for composite Simpson's rule can be approximated by

$$-\frac{h^4}{180}(f'''(b) - f'''(a)).$$

$$\begin{aligned}
E &= -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j) \\
&= -\frac{h^4}{180}\sum_{j=1}^{n/2} f^{(4)}(\xi_j)2h \\
&\stackrel{?}{=} -\frac{h^4}{180}\int_a^b f^{(4)}(x)dx \\
&= -\frac{h^4}{180}\left(f'''(b) - f'''(a)\right).
\end{aligned}$$

Recall. The Riemann integral of the function f on the interval $[a, b]$ is the following limit provided that it exists:

$$\int_a^b f(x)dx = \lim_{\max \Delta x_i \to 0} \sum_{i=1}^{n} f(z_i)\Delta x_i$$

where the numbers

$$x_0, x_1, \ldots, x_n$$

satisfy

$$a = x_0 \leq x_1 \leq \cdots \leq x_n = b,$$

and where

$$\Delta x_i = x_i - x_{i-1}$$

and z_i is arbitrarily chosen in the interval $[x_{i-1}, x_i]$ for $1 \leq i \leq n$.

Composite Integration – Stability

Assume that $f(x_i)$ is approximated by $\tilde{f}(x_i)$, and that

$$f(x_i) = \tilde{f}(x_i) + e_i, \quad \text{for each } i = 0, 1, \ldots, n,$$

where e_i denote the roundoff error associated with using $\tilde{f}(x_i)$ to approximate $f(x_i)$. In the Composite Simpson's rule:

$$\begin{aligned} e(h) &= \left| \frac{h}{3} \left(e_0 + 2 \sum_{j=1}^{n/2-1} e_{2j} + 4 \sum_{j=1}^{n/2} e_{2j-1} + e_n \right) \right| \\ &\le \frac{h}{3} \left(|e_0| + 2 \sum_{j=1}^{n/2-1} |e_{2j}| + 4 \sum_{j=1}^{n/2} |e_{2j-1}| + |e_n| \right). \end{aligned}$$

If the roundoff errors are *uniformly bounded* by ϵ, then

$$e(h) \leq \frac{h}{3}\left(\epsilon + 2\left(\frac{n}{2} - 1\right)\epsilon + 4\left(\frac{n}{2}\right)\epsilon + \epsilon\right) = nh\epsilon.$$

Since $nh = b - a$,

$$e(h) \leq (b - a)\epsilon,$$

which is independent of h and n. Hence, even though we may need to divide an interval into more parts to ensure accuracy, the increased computation does not increase the roundoff error. This implies that the method is *stable* as h approaches zero.

Romberg Integration

- Use the Composite Trapezoidal rule to obtain preliminary approximations;
- Apply the Richardson extrapolation process to improve the approximations.

Step 1: Preliminary Approximations

Trapezoidal rule with m subintervals:

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

$$a < \mu < b, \quad h = \frac{b-a}{m}, \quad x_j = a + jh, \; j = 0, 1, \ldots, m.$$

Initial Approximations $R_{k,1}$'s.

- Number of subintervals:

$$m_1 = 1,\ m_2 = 2,\ m_3 = 4,\ \ldots,\ m_n = 2^{n-1}.$$

- Step size h_k corresponding to m_k:

$$h_1 = b - a,\ h_2 = \frac{b-a}{2},\ h_3 = \frac{b-a}{4},\ h_k = \frac{b-a}{m_k} = \frac{b-a}{2^{k-1}}.$$

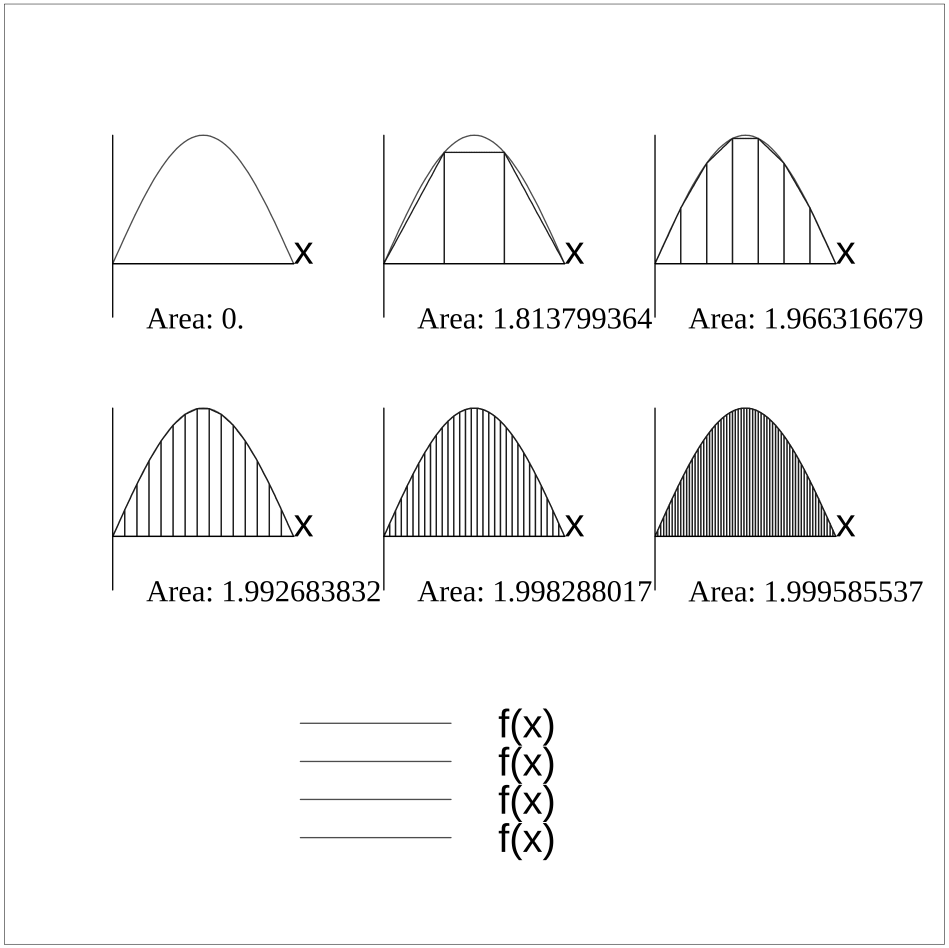
- Trapezoidal rule becomes:

$$\int_a^b f(x)dx \quad = \quad \underbrace{\frac{h_k}{2}\left(f(a) + f(b) + 2\left(\sum_{i=1}^{2^{k-1}-1} f(a) + ih_k)\right)\right)}_{R_{k,1}} -$$

$$\frac{b-a}{12} h_k^2 f''(\mu_k), \quad \mu_k \in (a,b).$$

$$
\begin{aligned}
R_{1,1} &= \frac{h_1}{2}\left(f(a)+f(b)\right) = \frac{b-a}{2}\left(f(a)+f(b)\right);\\
R_{2,1} &= \frac{h_2}{2}\left(f(a)+f(b)+2f(a+h_2)\right) = \frac{1}{2}(R_{1,1}+h_1 f(a+h_2));\\
R_{3,1} &= \frac{1}{2}(R_{2,1}+h_2(f(a+h_3)+f(a+3h_3)));\\
\dots &= \dots;\\
R_{k,1} &= \frac{1}{2}\left(R_{k-1,1}+h_{k-1}\sum_{i=1}^{2^{k-2}} f(a+(2i-1)h_k)\right).
\end{aligned}
$$

Example 1 Perform the first step of the Romberg integration scheme for approximating $\int_0^{\pi} \sin(x)dx$ with $n = 6$:


x
Area: 0.
Area: 1.813799364
Area: 1.966316679
Area: 1.992683832
Area: 1.998288017
Area: 1.999585537
f(x)
f(x)
f(x)
f(x)

Step 2: Richardson Extrapolation

- It can be shown that

$$\int_a^b f(x)dx - R_{k,1} = \sum_{i=1}^{\infty} K_i h_k^{2i} = K_1 h_k^2 + \sum_{i=2}^{\infty} K_i h_k^{2i}, \qquad (21)$$

  where K_i is independent of h_k, and depends only on $f^{(2i-1)}(a)$ and $f^{(2i-1)}(b)$.

- Replace h_k by $h_{k+1} = h_k/2$:

$$\begin{aligned} \int_a^b f(x)dx - R_{k+1,1} &= \sum_{i=1}^{\infty} K_i h_{k+1}^{2i} = \sum_{i=1}^{\infty} \frac{K_i h_k^{2i}}{2^{2i}} \\ &= \frac{K_1 h_k^2}{4} + \sum_{i=2}^{\infty} \frac{K_i h_k^{2i}}{2^{2i}} \qquad (22) \end{aligned}$$

- $4(22) - (21)$:

$$\int_a^b f(x)dx - \left(R_{k+1,1} + \frac{R_{k+1,1} - R_{k,1}}{3}\right) = \sum_{i=2}^{\infty} \frac{K_i}{3} \left(\frac{1 - 4^{i-1}}{4^{i-1}}\right) h_k^{2i}.$$

- In general, define

$$R_{k,2} = R_{k,1} + \frac{R_{k,1} - R_{k-1,1}}{3}, \quad k = 2, 3, \ldots, n,$$

apply Richardson extrapolation to these values. Continue this notation, for each $k = 2, 3, 4, \ldots, n$, and $j = 2, \ldots, k$, an $O\left(h_k^{2j}\right)$ approximation formula is defined by

$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}.$$

$$
\begin{array}{llllll}
\hline
R_{1,1} & & & & & \\
R_{2,1} & R_{2,2} & & & & \\
R_{3,1} & R_{3,2} & R_{3,3} & & & \\
R_{4,1} & R_{4,2} & R_{4,3} & R_{4,4} & & \\
\vdots & \vdots & \vdots & \vdots & & \\
R_{n,1} & R_{n,2} & R_{n,3} & R_{n,4} & \ldots & R_{n,n} \\
\hline
\end{array}
$$

A typical stopping criteria. Both $|R_{n-1,n-1} - R_{n,n}|$ and $|R_{n-2,n-2} - R_{n-1,n-1}|$ are within a desired tolerance.

Example 2 Given the initial approximations $R_{k,1}$, $1 \leq k \leq 6$ in Example 1, see textbook (Table 4.10, p.210) for the Romberg table.

Adaptive Quadrature

- Composite quadrature rules necessitate the use of *equally spaced* points. This does not take into account that some portions of the curve may have *large functional variations* that require more attention than other portions of the curve.
- It is useful to introduce a method that adjusts the step size to be smaller over portions of the curve where a larger functional variation occurs. This technique is called *adaptive quadrature*.
- We will discuss an adaptive quadrature based on Simpson's rule. The other composite procedures can be modified in a similar manner.

Adaptive Quadrature: a Sketch

Problem. Given $I_e = \int_a^b f(x)dx$. Approximate I_e to within a specified tolerance $\epsilon > 0$.

1. Simpson's $\longrightarrow \quad S(a,b)$,
2. Composite Simpson's $\longrightarrow \quad S(a,(a+b)/2),\ S((a+b)/2,b)$,
3. Using $S(a,b), S(a,(a+b)/2), S((a+b)/2,b)$, check if

$$\mathrm{Err}_{\mathrm{abs}} = \left| I_e - \left(S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right)\right)\right| < \epsilon.$$

   (a) Yes: Done.
   (b) No:
      i. $a := a,\ b := (a+b)/2$. Go to step 1. Check if $\mathrm{Err}_{\mathrm{abs}} < \epsilon/2$.
      ii. $a := (a+b)/2, b := b$. Go to step 1. Check if $\mathrm{Err}_{\mathrm{abs}} < \epsilon/2$.

Fill in the Details

- Apply Simpson's rule with step size $h = (b-a)/2$:

$$\int_a^b f(x)dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\mu), \quad \mu \in (a,b), \tag{23}$$

$$S(a,b) = \frac{h}{3}(f(a) + 4f(a+h) + f(b)).$$

- Apply composite Simpson's rule with $n = 4$, $h = (b-a)/4$:

$$\int_a^b f(x)dx = S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\tilde{\mu}), \tag{24}$$

$$S\left(a, \frac{a+b}{2}\right) = \frac{h}{6}\left(f(a) + 4f\left(a + \frac{h}{2}\right) + f(a+h)\right),$$

$$S\left(\frac{a+b}{2}, b\right) = \frac{h}{6}\left(f(a+h) + 4f\left(a + \frac{3h}{2}\right) + f(b)\right),$$

where $\tilde{\mu} \in (a,b)$.

ASSUMING THAT $\mu \approx \tilde{\mu}$, it follows from (23) and (24) that

$$\left|\int_a^b f(x)dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| \approx$$

$$\frac{1}{15} \underbrace{\left|S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right|}_{dS}.$$

If $dS < 15\epsilon$, then $\mathrm{Err}_{\mathrm{abs}} < \epsilon$, and

$$S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right)$$

is assumed to be a sufficiently accurate approximation to I_e.