Numerical Analysis

Lecture 11: Numerical Integration

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Outline

Numerical Integration

Quadrature based on interpolation polynomials

- The methods of quadrature in this section are based on the interpolation polynomials.
- The basic idea is to select a set of distinct nodes $x_0, \ldots, x_n$ from the interval $[a, b]$.
- Then integrate the Lagrange interpolating polynomial

$$P_n(x) = \sum_{i=0}^{n} f(x_i) L_i(x).$$

and its truncation error term over $[a, b]$ to obtain :

Numerical Integration

Quadrature based on interpolation polynomials (Cont'd)

$$\int_a^b f(x)dx = \int_a^b \sum_{i=0}^{n} f(x_i)L_i(x)dx + \int_a^b \prod_{i=0}^{n} (x - x_i)\frac{f^{(n+1)}(\xi(x))}{(n+1)!}dx$$
$$= \sum_{i=0}^{n} a_i f(x_i) + \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n} (x - x_i)f^{(n+1)}(\xi(x))dx$$

where $\xi(x)$ is in $[a, b]$ for each x and

$$a_i = \int_a^b L_i(x)dx$$

for each $i = 0, 1, ..., n$.

Numerical Integration

Quadrature based on interpolation polynomials (Cont'd)

The quadrature formula is, therefore,

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

where

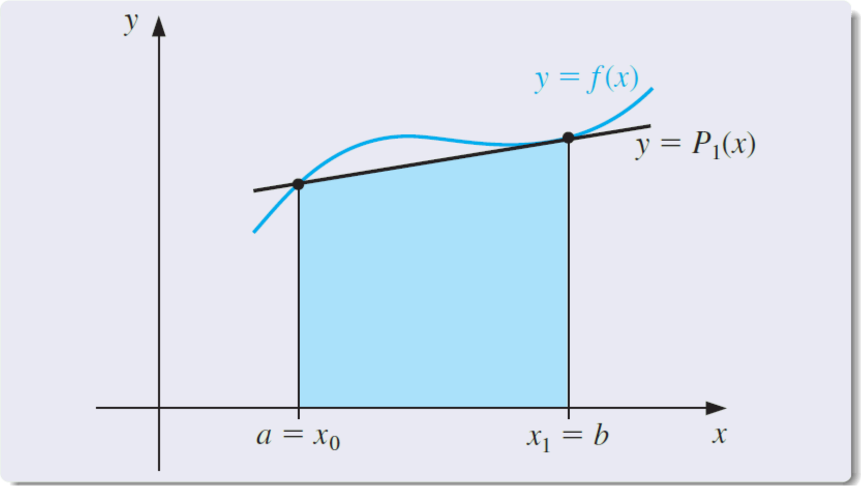
$$a_i = \int_a^b L_i(x)dx, \quad \text{for each } i = 0, 1, ..., n$$

and with error given by

$$E(f) = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^{n} (x - x_i) f^{(n+1)}(\xi(x))dx$$

Outline

Trapezoidal Rule



Trapezoidal Rule

Derivation(1/3)

To derive the Trapezoidal rule for approximating $\int_a^b f(x)dx$, let $x_0 = a, x_1 = b, h = b - a$ and use the linear Lagrange polynomial:

$$P_1(x) = \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1)$$

Then

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} \left[\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right] dx$$
$$+ \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)dx$$

Trapezoidal Rule

Derivation(2/3)

The product $(x-x_0)(x-x_1)$ does not change sign on $[x_0, x_1]$, so the Weighted Mean Value Theorem for Integrals can be applied to the error term to give, for some ξ in (x_0, x_1),

$$\begin{aligned}
&\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)dx \\
&= f''(\xi) \int_{x_0}^{x_1} (x-x_0)(x-x_1)dx \\
&= f''(\xi) \left[\frac{x^3}{3} - \frac{(x_1+x_0)}{2} x^2 + x_0 x_1 x \right]_{x_0}^{x_1} \\
&= -\frac{h^3}{6} f''(\xi)
\end{aligned}$$

Trapezoidal Rule

Derivation(3/3)

Consequently, the last equation, namely

$$\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)dx = -\frac{h^3}{6}f''(\xi)$$

implies that

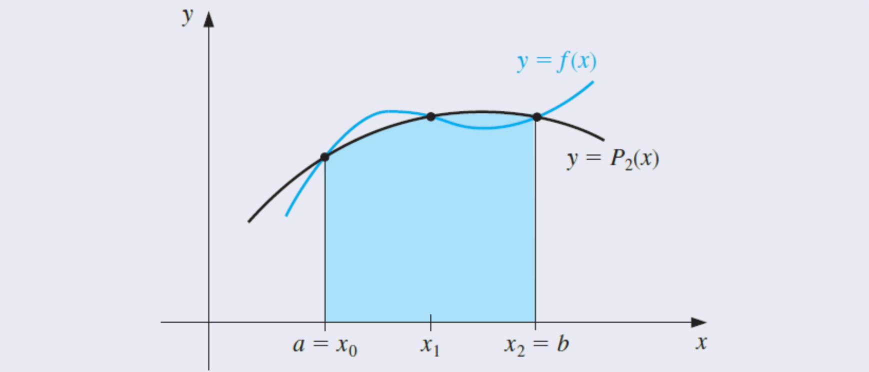
$$\int_a^b f(x)dx = \left[\frac{(x-x_1)^2}{2(x_0-x_1)}f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)}f(x_1)\right]_{x_0}^{x_1} - \frac{h^3}{12}f''(\xi)$$

$$= \frac{(x_1-x_0)}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12}f''(\xi)$$

Outline

Simpson's Rule

Simpson's rule results from integrating over $[a, b]$ the second Lagrange polynomial with equally-spaced nodes $x_0 = a, x_2 = b$, and $x_1 = a + h$, where $h = (b - a)/2$:



Simpson's Rule

Naive Derivation

Therefore

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \right.$$
$$\left. + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$
$$+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x))dx$$

- Deriving Simpson's rule in this manner, however, provides only an $O(h^4)$ error term involving $f^{(3)}$.
- By approaching the problem in another way, a higher-order term involving $f^{(4)}$ can be derived.

Simpson's Rule

Alternative Derivation (1/5)

Suppose that f is expanded in the third Taylor polynomial about x_1. Then for each x in $[x_0, x_2]$, a number $\xi(x)$ in (x_0, x_2) exists with

$$f(x) = f(x_1) + f'(x_1)(x - x_1) + \frac{f''(x_1)}{2}(x - x_1)^2 + \frac{f'''(x_1)}{6}(x - x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x - x_1)^4$$

and

$$\int_{x_0}^{x_2} f(x)dx = \left[f(x_1)(x - x_1) + \frac{f'(x_1)}{2}(x - x_1)^2 + \frac{f''(x_1)}{6}(x - x_1)^3 + \frac{f'''(x_1)}{24}(x - x_1)^4\right]_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4 dx$$

Simpson's Rule

Alternative Derivation (2/5)

Because $(x - x_1)^4$ is never negative on $[x_0, x_2]$, the Weighted Mean Value Theorem for Integrals implies that

$$\begin{aligned}\frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4 dx &= \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x - x_1)^4 dx \\ &= \frac{f^{(4)}(\xi_1)}{120}(x - x_1)^5\Big|_{x_0}^{x_2}\end{aligned}$$

for some number ξ_1 in (x_0, x_2).

Simpson's Rule

$$\frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4 dx = \frac{f^{(4)}(\xi_1)}{120}(x-x_1)^5\Big|_{x_0}^{x_2}$$

Alternative Derivation (3/5)

However, $h = x_2 - x_1 = x_1 - x_0$, so

$$(x_2-x_1)^2 - (x_0-x_1)^2 = (x_2-x_1)^4 - (x_0-x_1)^4 = 0$$

whereas

$$(x_2-x_1)^3 - (x_0-x_1)^3 = 2h^3 \text{ and } (x_2-x_1)^5 - (x_0-x_1)^5 = 2h^5$$

Simpson's Rule

Alternative Derivation (4/5)

Consequently,

$$\int_{x_0}^{x_2} f(x)dx = [f(x_1)(x - x_1) + \frac{f'(x_1)}{2}(x - x_1)^2 + \frac{f''(x_1)}{6}(x - x_1)^3 + \frac{f'''(x_1)}{24}(x - x_1)^4\Big|_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4 dx$$

can be re-written as

$$\int_{x_0}^{x_2} f(x)dx = 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \frac{f^{(4)}(\xi_1)}{60}h^5$$

Simpson's Rule

Alternative Derivation (5/5)

If we now replace $f''(x_1)$ by the approximation given by the Second Derivative Midpoint Formula, we obtain

$$\int_{x_0}^{x_2} f(x)dx = 2hf(x_1) + \frac{h^3}{3}\{\frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12}f^{(4)}(\xi_2)\} + \frac{f^{(4)}(\xi_1)}{60}h^5$$

$$= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{12}[\frac{1}{3}f^{(4)}(\xi_2) - \frac{1}{5}f^{(4)}(\xi_1)]$$

It can be shown by alternative methods that the values ξ_1 and ξ_2 in this expression can be replaced by a common value ξ in (x_0, x_2). This gives Simpson's rule.

Simpson's Rule

Simpson's Rule

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

The error term in Simpson's rule involves the fourth derivative of f, so it gives exact results when applied to any polynomial of degree three or less.

Simpson's Rule vs. Trapezoidal Rule

Example

Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^2 f(x)dx$ when $f(x)$ is

(a) x^2 (b) x^4 (c) $(x+1)^{-1}$
(d) $\sqrt{1+x^2}$ (e) $\sin x$ (f) e^x

Simpson's Rule vs. Trapezoidal Rule

Solution (1/3)

On $[0, 2]$, the Trapezoidal and Simpson's rule have the forms

Trapezoidal: $\int_0^2 f(x)dx \approx f(0) + f(2)$

Simpson's: $\int_0^2 f(x)dx \approx \frac{1}{3}[f(0) + 4f(1) + f(2)]$

When $f(x) = x^2$ they give

Trapezoidal: $\int_0^2 f(x)dx \approx 0^2 + 2^2 = 4$

Simpson's: $\int_0^2 f(x)dx \approx \frac{1}{3}[(0)^2 + 4 \cdot 1^2 + 2^2] = \frac{8}{3}$

Simpson's Rule vs. Trapezoidal Rule

Solution (2/3)

- The approximation from Simpson's rule is exact because its truncation error involves $f^{(4)}$, which is identically 0 when $f(x) = x^2$.
- The results to three places for the functions are summarized in the following table.

Simpson's Rule vs. Trapezoidal Rule

Solution(3/3): Summary Results

$f(x)$	(a) x^2	(b) x^4	(c) $(x+1)^{-1}$	(d) $\sqrt{1+x^2}$	(e) $\sin x$	(f) e^x
Exact value	2.667	6.400	1.099	2.958	1.416	6.389
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389
Simpson′s	2.667	6.667	1.111	2.964	1.425	6.421

Notice that, in each instance, Simpson's Rule is significantly superior.

Outline

Measuring Precision

Rationale

- The standard derivation of quadrature error formulas is based on determining the class of polynomials for which these formulas produce exact results.
- The following definition is used facilitate the discussion of this derivation.

Definition

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 $k = 0, 1, ..., n$

This implies that the Trapezoidal and Simpson's rules have degrees of precision one and three, respectively.

Measuring Precision

Degree of Precision

The degree of precision of a quadrature formula is n if and only if the error is zero for all polynomials of degree $k = 0, 1, ..., n$, but is not zero for some polynomial of degree $n + 1$.

Footnote

- The Trapezoidal and Simpson's rules are examples of a class of method known as Newton - Cotes formulas.
- There are two types of Newton - Cotes formulas, open and closed.

Closed Newton-Cotes Formulas

Closed Newton-Cotes Formulas

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$-point closed Newton-Cotes formulas with $x_0 = a, x_n = b$, and $h = (b-a)/n$. There exists $\xi \in (a,b)$ for which

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

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

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

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

Closed Newton-Cotes Formulas

- $n = 1$: Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12}f''(\xi)$$

- $n = 2$: Simpson's rule

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

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

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

- $n = 4$:

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

Outline

Composite Numerical Integration: Motivating Example

Application of Simpson's

Use Simpson's rule to approximate

$$\int_0^4 e^x$$

and compare this to the results obtained by adding the Simpson's rule approximations for

$$\int_0^2 e^x \quad \text{and} \quad \int_2^4 e^x$$

and adding those for

$$\int_0^1 e^x dx, \int_1^2 e^x dx, \int_2^3 e^x dx \ \text{ and } \ \int_3^4 e^x dx$$

Composite Numerical Integration: Motivating Example

Solution (1/3)

Simpson's rule on $[0, 4]$ uses $h = 2$ and gives

$$\int_0^4 e^x dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76958$$

The exact answer in this case is $e^4 - e^0 = 53.59815$, and the error -3.17143 is far larger than we could normally accept.

Solution (2/3)

Applying Simpson's rule on each of the intervals $[0, 2]$ and $[2, 4]$ uses $h = 1$ and gives

$$\begin{aligned}\int_0^4 e^x dx &= \int_0^2 e^x dx + \int_2^4 e^x dx \\ &\approx \frac{1}{3}(e^0 + 4e + e^2) + \frac{1}{3}(e^2 + 4e^3 + e^4) \\ &= \frac{1}{3}(e^0 + 4e + 2e^2 + 4e^3 + e^4) \\ &= 53.86385\end{aligned}$$

The error has been reduced to -0.26570.

Composite Numerical Integration: Motivating Example

Solution (3/3)

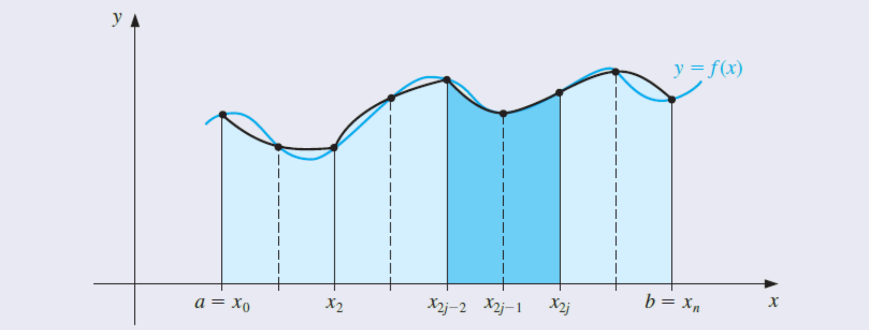
For the integrals on $[0, 1]$, $[1, 2]$, $[2, 3]$, and $[3, 4]$ we use Simpson's rule four times with $h = \dfrac{1}{2}$ giving

$$\int_0^4 e^x dx = \int_0^1 e^x dx + \int_1^2 e^x dx + \int_2^3 e^x dx + \int_3^4 e^x dx$$
$$\approx \frac{1}{6}(e^0 + 4e^{1/2} + e) + \frac{1}{6}(e + 4e^{3/2} + e^2)$$
$$+ \frac{1}{6}(e^2 + 4e^{5/2} + e^3) + \frac{1}{6}(e^3 + 4e^{7/2} + e^4)$$
$$= \frac{1}{6}(e^0 + 4e^{1/2} + 2e + 4e^{3/2} + 2e^2 + 4e^{5/2} + 2e^3 + 4e^{7/2} + e^4)$$
$$= 53.61622$$

The error for this approximation has been reduced to - 0.01807.

Composite Numerical Integration: Simpson's Rule

To generalize this procedure for an arbitrary integral $\int_a^b f(x)dx$, choose an even integer n. Subdivide the interval $[a, b]$ into n subintervals, and apply Simpson's rule on each consecutive pair of subintervals.



Composite Numerical Integration: Simpson's Rule

Construct the Formula & Error Term

With $h = (b-a)/n$ and $x_j = a + jh$, for each $j = 1, 2, ..., n$, we have

$$\int_a^b f(x)dx = \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)dx$$
$$= \sum_{j=1}^{n/2} \{\frac{h}{3}[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})] - \frac{h^5}{90} \sum_{j=1}^{(n/2)} f^{(4)}(\xi_j)\}$$

for some ξ_j with $x_{2j-2} < \xi_j < x_{2j}$, provided that $f \in C^4[a,b]$.

Composite Numerical Integration: Simpson's Rule

$$\int_a^b f(x)dx = \sum_{j=1}^{n/2} \{\frac{h}{3}[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})] - \frac{h^5}{90}f^{(4)}(\xi_j)\}$$

Construct the Formula & Error Term (Cont'd)

Using the fact that for each $j = 1, 2, ..., (n/2) - 1$ we have $f(x_{2j})$ appearing in the term corresponding to the interval $[x_{2j-2}, x_{2j}]$ and also in the term corresponding to the interval $[x_{2j}, x_{2j+2}]$, we can reduce this sum to

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(x_0) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{(n/2)} f(x_{2j-1}) + f(x_n)\right] - \frac{h^5}{90}\sum_{j=1}^{(n/2)} f^{(4)}(\xi_j)$$

Composite Numerical Integration: Simpson's Rule

Construct the Formula & Error Term (Cont'd)

The error associated with this approximation is

$$E(f) = -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j)$$

where $x_{2j-2} < \xi_j < x_{2j}$, for each $j = 1, 2, ..., n/2$. If $f \in C^4[a, b]$, the Extreme Value Theorem implies that $f^{(4)}$ assumes its maximum and minimum in $[a, b]$.

Composite Numerical Integration: Simpson's Rule

Construct the Formula & Error Term (Cont'd)

Since

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

we have

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

and

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

Construct the Formula & Error Term (Cont'd)

By the Intermediate Value Theorem there is a $\mu \in (a, b)$ such that

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

Thus

$$E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) = -\frac{h^5}{180} n f^{(4)}(\mu)$$

or, since $h = (b - a)/n$

$$E(f) = -\frac{(b-a)}{180} h^4 f^{(4)}(\mu)$$

Composite Numerical Integration: Simpson's Rule

Theorem (Composite Simpson's Rule)

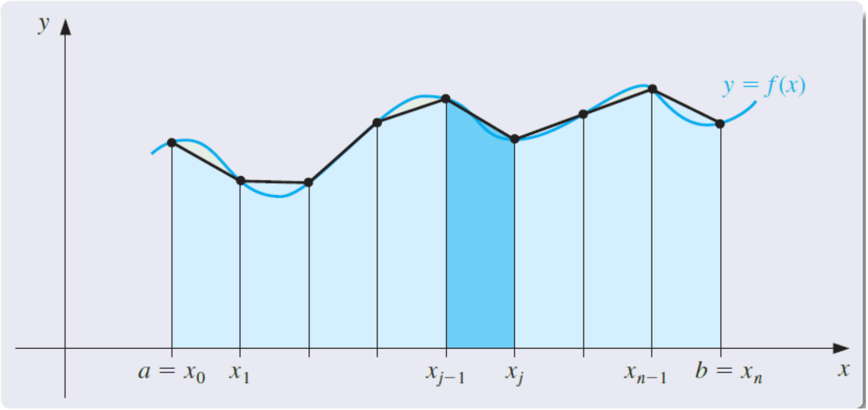
Let $f \in C^4[a, b]$, n be even, $h = (b - a)/n$, and $x_j = a + jh$, for each $j = 0, 1, ..., n$. These exists a $\mu \in (a, b)$ for which the Composite Simpson's rule for n subintervals can be written with its error term as

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

Comments on the Formula & Error Term

- Notice that the error term for the Composite Simpson's rule is $O(h^4)$, whereas it was $O(h^5)$ for the standard Simpson's rule.
- However, these rates are not comparable because, for the standard Simpson's rule, we have h fixed at $h = (b - a)/2$, but for Composite Simpson's rule we have $h = (b - a)/n$, for n an even integer.
- This permits us to considerably ruduce the value of h.
- The following algorithm uses the Composite Simpson's rule on n subintervals. It is the most frequently-used general-purpose quadrature algorithm.

Composite Trapezoidal Rule



Note: The Trapezoidal rule requires only one interval for each application, so the integer n can be either odd or even.

Composite Trapezoidal Rule

Theorem (Composite Trapezoidal Rule)

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

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

Round-Off Error Stability

- More round-off error may be involved if more computation is needed.
- However, for the Composite Rule, round-off error does not depend on the number of calculations performed.

$$f(x_i) = \tilde{f}(x_i) + e_i$$

$$e(h) \leq \frac{h}{3}[\varepsilon + 2(n/2 - 1)\varepsilon + 4(n/2)\varepsilon + \varepsilon] = nh\varepsilon = (b-a)\varepsilon$$

Outline

Basic Romberg Method

Composite Trapezoidal Rule: Error Term

- We will illustrate how Richardson extrapolation applied to results from the Composite Trapezoidal rule can be used to obtain high accuracy approximations with little computational cost
- We have seen that the Composite Trapezoidal rule has a truncation error of order $O(h^2)$. Specifically, we showed that for $h = (b-a)/n$ and $x_j = a + jh$ we have

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

for some number μ in(a, b).

Basic Romberg Method

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

Composite Trapezoidal Rule: Error Term (Cont'd)

By an alternative method, it can be shown that if $f \in C^\infty[a,b]$,the Composite Trapezoidal rule can also be written with an error term in the form

$$\int_a^b f(x)dx = \frac{h}{2}[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)] + K_1h^2 + K_2h^4 + K_3h^6 + \ldots$$

where each K_i is a constant that depends only on $f^{(2i-1)}(a)$ and $f^{(2i-1)}(b)$.

Basic Romberg Method

$$\int_a^b f(x)dx = \frac{h}{2}[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)] + K_1h^2 + K_2h^4 + K_3h^6 + \dots$$

Applying Richardson Extrapolation

- We have seen that Richardson extrapolation can be performed on any approximation procedure whose truncation error is of the form

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

for a collection of constants K_j and when

$$\alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_m.$$

Basic Romberg Method

Applying Richardson Extrapolation (Cont'd)

- To approximate the integral $\int_a^b f(x)dx$ we use the results of the Composite Trapezoidal Rule with $n = 1, 2, 4, 8, 16, \ldots$, and denote the resulting approximations, respectively, by $R_{1,1}, R_{2,1}, R_{3,1}$, etc
- We then apply extrapolation in the manner seen before, that is, we obtain $O(h^4)$ approximations $R_{2,2}, R_{3,2}, R_{4,2}$, etc, by

$$R_{k,2} = R_{k,1} + \frac{1}{3}(R_{k,1} - R_{k-1,1}), \text{ for } k = 2, 3, \ldots$$

and $O(h^6)$ approximations $R_{3,3}, R_{4,3}, R_{5,3}$, etc, by

$$R_{k,3} = R_{k,2} + \frac{1}{15}(R_{k,2} - R_{k-1,2}), \text{ for } k = 3, 4, \ldots$$

Basic Romberg Method

Romberg Integration

In general, after the appropriate $R_{k,j-1}$ approximations have been obtained, we determine the $O(h^{2j})$ approximations from

$$R_{k,j} = R_{k,j-1} + \frac{1}{4^{j-1}-1}(R_{k,j-1} - R_{k-1,j-1}), \text{ for } k = j, j+1, \cdots$$

Basic Romberg Method

Example: Composite Trapezoidal & Romberg

- Use the Composite Trapezoidal rule to find approximations to $\int_0^{\pi} \sin x dx$ with $n = 1,\ 2,\ 4,\ 8,$ and 16
- Then perform Romberg extrapolation on the results.

Basic Romberg Method

Solution (1/6): Composite Trapezoidal Rule Approximations

The Composite Trapezoidal rule for the various values of n gives the following approximations to the true value 2.

$$R_{1,1} = \frac{\pi}{2}[\sin 0 + \sin \pi] = 0$$

$$R_{2,1} = \frac{\pi}{4}[\sin 0 + 2\sin\frac{\pi}{2} + \sin \pi] = 1.57079633$$

$$R_{3,1} = \frac{\pi}{8}[\sin 0 + 2(\sin\frac{\pi}{4} + \sin\frac{\pi}{2} + \sin\frac{3\pi}{4}) + \sin \pi]$$

$$= 1.89611890$$

Basic Romberg Method

Solution (2/6): Composite Trapezoidal Rule Approximations

$$R_{4,1} = \frac{\pi}{16}[\sin 0 + 2(\sin \frac{\pi}{8} + \sin \frac{\pi}{4} + \ldots + \sin \frac{3\pi}{4} + \sin \frac{7\pi}{8}) + \sin \pi] = 1.97423160$$

$$R_{5,1} = \frac{\pi}{32}[\sin 0 + 2(\sin \frac{\pi}{16} + \sin \frac{\pi}{8} + \ldots + \sin \frac{7\pi}{8} + \sin \frac{15\pi}{16}) + \sin \pi] = 1.99357034$$

Basic Romberg Method

Solution (3/6): Romberg Extrapolation

The $O(h^4)$ approximations are

$$
\begin{aligned}
R_{2,2} &= R_{2,1} + \frac{1}{3}(R_{2,1} - R_{1,1}) = 2.09439511 \\
R_{3,2} &= R_{3,1} + \frac{1}{3}(R_{3,1} - R_{2,1}) = 2.00455976 \\
R_{4,2} &= R_{4,1} + \frac{1}{3}(R_{4,1} - R_{3,1}) = 2.00026917 \\
R_{5,2} &= R_{5,1} + \frac{1}{3}(R_{5,1} - R_{4,1}) = 2.00001659
\end{aligned}
$$

Basic Romberg Method

Solution (4/6): Romberg Extrapolation

The $O(h^6)$ approximations are

$$\begin{aligned} R_{3,3} &= R_{3,2} + \frac{1}{15}(R_{3,2} - R_{2,2}) = 1.99857073 \\ R_{4,3} &= R_{4,2} + \frac{1}{15}(R_{4,2} - R_{3,2}) = 1.99998313 \\ R_{5,3} &= R_{5,2} + \frac{1}{15}(R_{5,2} - R_{4,2}) = 1.99999975 \end{aligned}$$

Basic Romberg Method

Solution (5/6): Romberg Extrapolation

The two $O(h^8)$ approximations are

$$R_{4,4} = R_{4,3} + \frac{1}{63}(R_{4,3} - R_{3,3}) = 2.00000555$$
$$R_{5,4} = R_{5,3} + \frac{1}{63}(R_{5,3} - R_{4,3}) = 2.00000001$$

and the final $O(h^{10})$ approximations is

$$R_{5,5} = R_{5,4} + \frac{1}{255}(R_{5,4} - R_{4,4}) = 1.99999999$$

These results are shown in the following table

Solution (6/6): Romberg Extrapolation

0				
1.57079633	2.09439511			
1.89611890	2.00455976	1.99857073		
1.97423160	2.00026917	1.99998313	2.00000555	
1.99357034	2.00001659	1.99999975	2.00000001	1.99999999

Romberg Integration: Recursive Calculation

Romberg Method

Extrapolation then is used to produce $O(h_k^{2j})$ approximations by

Romberg Method

$$R_{k,j} = R_{k,j-1} + \frac{1}{4^{j-1} - 1}\left(R_{k,j-1} - R_{k-1,j-1}\right)$$

for $k = j, j+1, \cdots$.

as shown in the following table.

Romberg Integration: Recursive Calculation

Approximating a Derivative

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

for $k = j, j+1, \ldots.$

The Romberg Table

k	$O(h_k^2)$	$O(h_k^4)$	$O(h_k^6)$	$O(h_k^8)$		$O(h_k^{2n})$
1	$R_{1,1}$					
2	$R_{2,1}$	$R_{2,2}$				
3	$R_{3,1}$	$R_{3,2}$	$R_{3,3}$			
4	$R_{4,1}$	$R_{4,2}$	$R_{4,3}$	$R_{4,4}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
n	$R_{n,1}$	$R_{n,2}$	$R_{n,3}$	$R_{n,4}$	$\ldots$	$R_{n,n}$

Romberg Integration: Recursive Calculation

To approximate the integral $I = \int_a^b f(x)\,dx$, select an integer $n > 0$.

INPUT	endpoints a, b; integer n.
OUTPUT	an array R (compute R by rows; only the last 2 rows are saved in storage).
Step 1	Set $h = b - a$ $R_{1,1} = \frac{h}{2}(f(a) + f(b))$
Step 2	OUTPUT $(R_{1,1})$

Steps 3 to 9 are on the next slide

Romberg Integration: Recursive Calculation

Step 3 For $i = 2, \ldots, n$ do Steps 4–8:

Step 4

$$\text{Set } R_{2,1} = \frac{1}{2}\left[R_{1,1} + h\sum_{k=1}^{2^{i-2}} f(a + (k - 0.5)h)\right]$$

(Approximation from the Trapezoidal method)

Step 5 For $j = 2, \ldots, i$

$$\text{set } R_{2,j} = R_{2,j-1} + \frac{R_{2,j-1} - R_{1,j-1}}{4^{j-1} - 1} \quad \textit{(Extrapolation)}$$

Step 6 OUTPUT ($R_{2,j}$ for $j = 1, 2, \ldots, i$)

Step 7 Set $h = h/2$

Step 8 For $j = 1, 2, \ldots, i$ set $R_{1,j} = R_{2,j}$

(*Update row 1 of R*)

Step 9 STOP

Romberg Integration Algorithm

Comments on the Algorithm (1/2)

- The algorithm requires a preset integer n to determine the number of rows to be generated.
- We could also set an error tolerance for the approximation and generate n, within some upper bound, until consecutive diagonal entries $R_{n-1,n-1}$ and $R_{n,n}$ agree to within the tolerance.

Romberg Integration Algorithm

Comments on the Algorithm (2/2)

- To guard against the possibility that two consecutive row elements agree with each other but not with the value of the integral being approximated, it is common to generate approximations until not only

$$|R_{n-1,n-1} - R_{n,n}|$$

is within the tolerance, but also

$$|R_{n-2,n-2} - R_{n-1,n-1}|$$

- Although not a universal safeguard, this will ensure that two differently generated sets of approximations agree within the specified tolerance before $R_{n,n}$, is accepted as sufficiently accurate.

Assignment

- Reading Assignment: Chap 4.3-4.5
- Homework: Assignment 5