Numerical Differentiation & Integration

Elements of Numerical Integration I

Numerical Analysis (9th Edition)

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Outline

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Introduction to Numerical Integration

Numerical Quadrature

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- The need often arises for evaluating the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to obtain.

Introduction to Numerical Integration

Numerical Quadrature

- The need often arises for evaluating the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to obtain.
- The basic method involved in approximating $\int_a^b f(x)\,dx$ is called numerical quadrature. It uses a sum $\sum_{i=0}^{n} a_i f(x_i)$ to approximate $\int_a^b f(x)\,dx$.

Introduction to Numerical Integration

Quadrature based on interpolation polynomials

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Introduction to 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:

Introduction to Numerical Integration

Quadrature based on interpolation polynomials (Cont'd)

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

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

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

Introduction to Numerical Integration

Quadrature based on interpolation polynomials (Cont'd)

The quadrature formula is, therefore,

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

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Introduction to Numerical Integration

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where

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

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

Numerical Integration: Trapezoidal Rule

Derivation (1/3)

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Numerical Integration: Trapezoidal Rule

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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:

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

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

Then

$$\begin{aligned}\int_a^b f(x)\,dx \;&=\; \int_{x_0}^{x_1} \left[\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right] dx \\ &\quad + \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\,dx.\end{aligned}$$

Numerical Integration: 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 See Theorem can be applied to the error term

Numerical Integration: 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 ▸ See Theorem can be applied to the error term to give, for some ξ in (x_0, x_1),

$$\begin{aligned} & \int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\, dx \\ = \quad & f''(\xi) \int_{x_0}^{x_1} (x - x_0)(x - x_1)\, dx \end{aligned}$$

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

Numerical Integration: Trapezoidal Rule

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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 See Theorem can be applied to the error term to give, for some ξ in (x_0, x_1),

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

Numerical Integration: Trapezoidal Rule

Derivation (3/3)

Consequently, the last equation, namely

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

Numerical Integration: Trapezoidal Rule

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Consequently, the last equation, namely

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implies that

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

Numerical Integration: Trapezoidal Rule

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Consequently, the last equation, namely

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implies that

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

Numerical Integration: Trapezoidal Rule

Using the notation $h = x_1 - x_0$ gives the following rule:

The Trapezoidal Rule

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

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Note:

- The error term for the Trapezoidal rule involves f'', so the rule gives the exact result when applied to any function whose second derivative is identically zero, that is, any polynomial of degree one or less.

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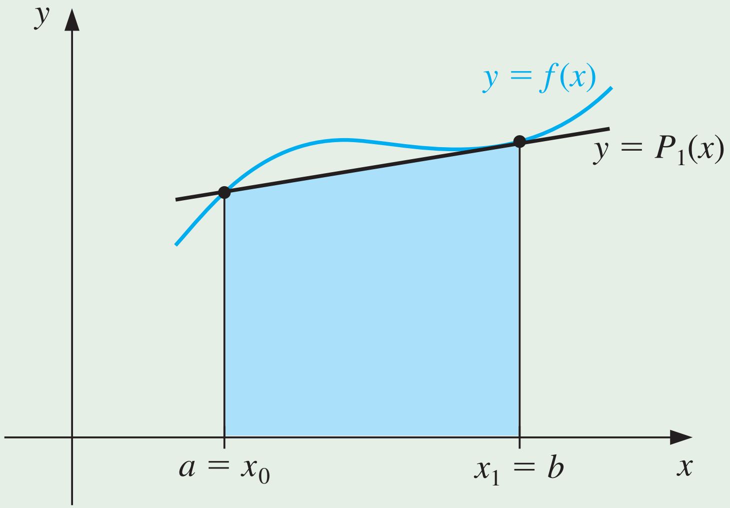
Note:

- The error term for the Trapezoidal rule involves f'', so the rule gives the exact result when applied to any function whose second derivative is identically zero, that is, any polynomial of degree one or less.
- The method is called the Trapezoidal rule because, when f is a function with positive values, $\int_a^b f(x)\,dx$ is approximated by the area in a trapezoid, as shown in the following diagram.

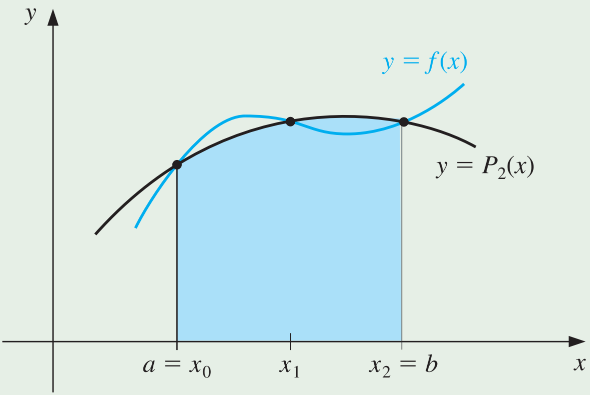
Trapezoidal Rule: The Area in a Trapezoid



Outline

Numerical Integration: 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 $h = (b - a)/2$:



Numerical Integration: Simpson's Rule

Naive Derivation

Numerical Integration: Simpson's Rule

Naive Derivation

Therefore

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

Numerical Integration: Simpson's Rule

Naive Derivation

Therefore

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

Deriving Simpson's rule in this manner, however, provides only an $O(h^4)$ error term involving $f^{(3)}$.

Numerical Integration: Simpson's Rule

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

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.

Numerical Integration: Simpson's Rule

Alternative Derivation (1/5)

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

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and

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

Numerical Integration: Simpson's Rule

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$$\frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4\,dx \quad = \quad \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x-x_1)^4\,dx$$

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

for some number ξ_1 in (x_0, x_2).

Numerical Integration: Simpson's Rule

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Alternative Derivation (3/5)

Numerical Integration: Simpson's Rule

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Alternative Derivation (3/5)

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

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

Numerical Integration: Simpson's Rule

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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

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

Numerical Integration: Simpson's Rule

Alternative Derivation (4/5)

Numerical Integration: Simpson's Rule

Alternative Derivation (4/5)

Consequently,

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

Numerical Integration: Simpson's Rule

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Consequently,

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can be re-written as

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

Numerical Integration: Simpson's Rule

Alternative Derivation (5/5)

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

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

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$$\begin{aligned}\int_{x_0}^{x_2} f(x)\,dx &= 2hf(x_1) + \frac{h^3}{3}\left\{\frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12}f^{(4)}(\xi_2)\right\} \\ &\qquad + \frac{f^{(4)}(\xi_1)}{60}h^5 \\ &= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{12}\left[\frac{1}{3}f^{(4)}(\xi_2) - \frac{1}{5}f^{(4)}(\xi_1)\right]\end{aligned}$$

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$$\begin{aligned}\int_{x_0}^{x_2} f(x)\,dx &= 2hf(x_1) + \frac{h^3}{3}\left\{\frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12}f^{(4)}(\xi_2)\right\} \\ &\qquad + \frac{f^{(4)}(\xi_1)}{60}h^5 \\ &= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{12}\left[\frac{1}{3}f^{(4)}(\xi_2) - \frac{1}{5}f^{(4)}(\xi_1)\right]\end{aligned}$$

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.

Numerical Integration: 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.

Outline

Trapezoidal Rule .v. Simpson's 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

Trapezoidal Rule .v. Simpson's Rule

Solution (1/3)

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

$$\text{Trapezoidal:} \quad \int_0^2 f(x)\,dx \approx f(0) + f(2)$$

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

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

$$\text{Trapezoidal:} \quad \int_0^2 f(x)\, dx \approx 0^2 + 2^2 = 4$$

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

Trapezoidal Rule .v. Simpson's Rule

Solution (2/3)

- The approximation from Simpson's rule is exact because its truncation error involves $f^{(4)}$, which is identically 0 when $f(x) = x^2$.

Trapezoidal Rule .v. Simpson's 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.

Trapezoidal Rule .v. Simpson's Rule

Solution (3/3): Summary Results

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

Numerical Integration: Measuring Precision

Rationale

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

Numerical Integration: Measuring Precision

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

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

Numerical Integration: Measuring Precision

Establishing the Degree of Precision

Numerical Integration: Measuring Precision

Establishing the Degree of Precision

Integration and summation are linear operations; that is,

$$\int_a^b (\alpha f(x) + \beta g(x))\, dx = \alpha \int_a^b f(x)\, dx + \beta \int_a^b g(x)\, dx$$

and

$$\sum_{i=0}^{n} (\alpha f(x_i) + \beta g(x_i)) = \alpha \sum_{i=0}^{n} f(x_i) + \beta \sum_{i=0}^{n} g(x_i),$$

for each pair of integrable functions f and g and each pair of real constants α and β.

Numerical Integration: Measuring Precision

Establishing the Degree of Precision

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for each pair of integrable functions f and g and each pair of real constants α and β. This implies the following:

Numerical Integration: 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 $k = 0, 1, \ldots, n$, but is not zero for some polynomial of degree $n + 1$.

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Footnote

- The Trapezoidal and Simpson's rules are examples of a class of methods known as Newton-Cotes formulas.

Numerical Integration: Measuring Precision

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Footnote

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

Questions?

Reference Material

The Weighted Mean Value Theorem for Integrals

- Suppose $f \in C[a,b]$, the Riemann integral of g exists on $[a,b]$, and $g(x)$ does not change sign on $[a,b]$. Then there exists a number c in (a,b) with

$$\int_a^b f(x)g(x)\,dx = f(c)\int_a^b g(x)\,dx.$$

- When $g(x) \equiv 1$, this result is the usual Mean Value Theorem for Integrals. It gives the average value of the function f over the interval $[a,b]$ as

$$f(c) = \frac{1}{b-a}\int_a^b f(x)\,dx.$$

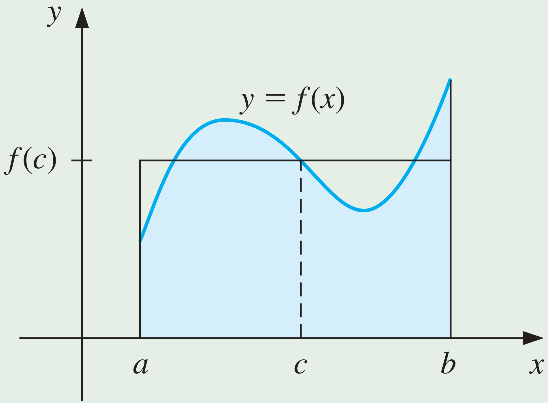
See Diagram

Return to Derivation of the Trapezoidal Rule
Return to Derivation of Simpson's Method

The Mean Value Theorem for Integrals

$$f(c) = \frac{1}{b-a} \int_a^b f(x)\, dx.$$

Return to the Weighted Mean Value Theorem for Integrals



Numerical Differentiation Formulae

Second Derivative Midpoint Formula

$$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12}f^{(4)}(\xi)$$

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

Return to Derivation of Simpson's Rule