Numerical Differentiation & Integration

Numerical Differentiation I

Numerical Analysis (9th Edition)

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Outline

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1. Introduction to Numerical Differentiation
2. General Derivative Approximation Formulas

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3. Some useful three-point formulas

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Introduction to Numerical Differentiation

Approximating a Derivative

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- The derivative of the function f at x_0 is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}.$$

Introduction to Numerical Differentiation

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- This formula gives an obvious way to generate an approximation to $f'(x_0)$; simply compute

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for small values of h. Although this may be obvious, it is not very successful, due to our old nemesis round-off error.

Introduction to Numerical Differentiation

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for small values of h. Although this may be obvious, it is not very successful, due to our old nemesis round-off error.

- But it is certainly a place to start.

Introduction to Numerical Differentiation

Approximating a Derivative (Cont'd)

- To approximate $f'(x_0)$, suppose first that $x_0 \in (a, b)$, where $f \in C^2[a, b]$, and that $x_1 = x_0 + h$ for some $h \neq 0$ that is sufficiently small to ensure that $x_1 \in [a, b]$.

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- We construct the first Lagrange polynomial $P_{0,1}(x)$ for f determined by x_0 and x_1, with its error term:

$$f(x) = P_{0,1}(x) + \frac{(x - x_0)(x - x_1)}{2!} f''(\xi(x))$$

$$= \frac{f(x_0)(x - x_0 - h)}{-h} + \frac{f(x_0 + h)(x - x_0)}{h} + \frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi(x))$$

for some $\xi(x)$ between x_0 and x_1.

Numerical Differentiation

$$f(x) = \frac{f(x_0)(x - x_0 - h)}{-h} + \frac{f(x_0 + h)(x - x_0)}{h} + \frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi(x))$$

Differentiating gives

$$f'(x) = \frac{f(x_0 + h) - f(x_0)}{h} + D_x \left[\frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi(x)) \right]$$

Numerical Differentiation

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Numerical Differentiation

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Deleting the terms involving $\xi(x)$ gives

$$f'(x) \approx \frac{f(x_0 + h) - f(x_0)}{h}$$

Numerical Differentiation

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Approximating a Derivative (Cont'd)

- One difficulty with this formula is that we have no information about $D_x f''(\xi(x))$, so the truncation error cannot be estimated.

Numerical Differentiation

$$f'(x) \approx \frac{f(x_0 + h) - f(x_0)}{h}$$

Approximating a Derivative (Cont'd)

- One difficulty with this formula is that we have no information about $D_x f''(\xi(x))$, so the truncation error cannot be estimated.
- When x is x_0, however, the coefficient of $D_x f''(\xi(x))$ is 0, and the formula simplifies to

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi)$$

Numerical Differentiation

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi)$$

Forward-Difference and Backward-Difference Formulae

- For small values of h, the difference quotient

$$\frac{f(x_0 + h) - f(x_0)}{h}$$

can be used to approximate $f'(x_0)$ with an error bounded by $M|h|/2$, where M is a bound on $|f''(x)|$ for x between x_0 and $x_0 + h$.

Numerical Differentiation

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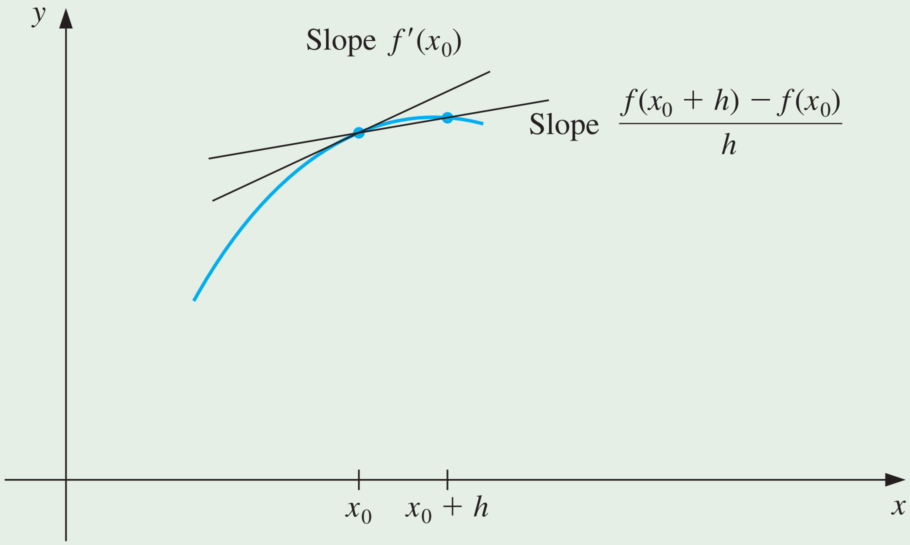
  can be used to approximate $f'(x_0)$ with an error bounded by $M|h|/2$, where M is a bound on $|f''(x)|$ for x between x_0 and x_0+h.
- This formula is known as the forward-difference formula if $h > 0$ and the backward-difference formula if $h < 0$.

Forward-Difference Formula to Approximate $f'(x_0)$



Numerical Differentiation

Example 1: $f(x) = \ln x$

Use the forward-difference formula to approximate the derivative of $f(x) = \ln x$ at $x_0 = 1.8$ using $h = 0.1$, $h = 0.05$, and $h = 0.01$, and determine bounds for the approximation errors.

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Solution (1/3)

The forward-difference formula

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

with $h = 0.1$

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The forward-difference formula

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

with $h = 0.1$ gives

$$\frac{\ln 1.9 - \ln 1.8}{0.1} = \frac{0.64185389 - 0.58778667}{0.1} = 0.5406722$$

Numerical Differentiation: Example 1

Solution (2/3)

Because $f''(x) = -1/x^2$ and $1.8 < \xi < 1.9$, a bound for this approximation error is

$$\frac{|hf''(\xi)|}{2} = \frac{|h|}{2\xi^2} < \frac{0.1}{2(1.8)^2} = 0.0154321$$

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The approximation and error bounds when $h = 0.05$ and $h = 0.01$ are found in a similar manner and the results are shown in the following table.

Numerical Differentiation: Example 1

Solution (3/3): Tabulated Results

h	$f(1.8+h)$	$\dfrac{f(1.8+h)-f(1.8)}{h}$	$\dfrac{\lvert h \rvert}{2(1.8)^2}$
0.1	0.64185389	0.5406722	0.0154321
0.05	0.61518564	0.5479795	0.0077160
0.01	0.59332685	0.5540180	0.0015432

Since $f'(x) = 1/x$ The exact value of $f'(1.8)$ is $0.55\overline{5}$, and in this case the error bounds are quite close to the true approximation error.

Outline

General Derivative Approximation Formulas

Method of Construction

- To obtain general derivative approximation formulas, suppose that $\{x_0, x_1, \ldots, x_n\}$ are $(n+1)$ distinct numbers in some interval I and that $f \in C^{n+1}(I)$.
- From the interpolation error theorem ▸ Theorem we have

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

for some $\xi(x)$ in I, where $L_k(x)$ denotes the kth Lagrange coefficient polynomial for f at $x_0, x_1, \ldots, x_n$.

General Derivative Approximation Formulas

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

Method of Construction (Cont'd)

Differentiating this expression gives

$$f'(x) = \sum_{k=0}^{n} f(x_k)L_k'(x) + D_x\left[\frac{(x-x_0)\cdots(x-x_n)}{(n+1!)}\right] f^{(n+1)}(\xi(x))$$
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General Derivative Approximation Formulas

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We again have a problem estimating the truncation error unless x is one of the numbers x_j.

General Derivative Approximation Formulas

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Method of Construction (Cont'd)

We again have a problem estimating the truncation error unless x is one of the numbers x_j. In this case, the term multiplying $D_x[f^{(n+1)}(\xi(x))]$ is 0, and the formula becomes

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L'_k(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{\substack{k=0 \\ k\neq j}}^{n} (x_j - x_k)$$

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which is called an $\boldsymbol{(n+1)}$**-point formula** to approximate $f'(x_j)$.

General Derivative Approximation Formulas

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Comment on the $(n+1)$-point formula

- In general, using more evaluation points produces greater accuracy, although the number of functional evaluations and growth of round-off error discourages this somewhat.

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- The most common formulas are those involving three and five evaluation points.

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We first derive some useful three-point formulas and consider aspects of their errors.

Outline

Some useful three-point formulas

Important Building Blocks

Since

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}$$

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we obtain

$$L_0'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}$$

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we obtain

$$L_0'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}$$

In a similar way, we find that

$$L_1'(x) = \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}$$

$$L_2'(x) = \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$$

Some useful three-point formulas

Important Building Blocks (Cont'd)

Using these expressions for $L_j'(x)$, $1 \leq j \leq 2$, the $n+1$-point formula

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

Some useful three-point formulas

Important Building Blocks (Cont'd)

Using these expressions for $L'_j(x)$, $1 \le j \le 2$, the $n+1$-point formula

$$f'(x_j) = \sum_{k=0}^{n} f(x_k) L'_k(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{\substack{k=0 \\ k \ne j}}^{n} (x_j - x_k)$$

becomes for $n = 2$:

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

for each $j = 0, 1, 2$, where $\xi_j = \xi_j(x)$.

Some useful three-point formulas

$$f'(x_j) = f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right] + f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right] + f(x_2)\left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}\right] + \frac{1}{6}f^{(3)}(\xi_j)\prod_{\substack{k=0 \\ k\neq j}}^{2}(x_j - x_k)$$

Assumption

Some useful three-point formulas

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

Assumption

The 3-point formulas become especially useful if the nodes are equally spaced, that is, when

$$x_1 = x_0 + h \quad \text{and} \quad x_2 = x_0 + 2h, \quad \text{for some } h \neq 0$$

Some useful three-point formulas

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We will assume equally-spaced nodes throughout the remainder of this section.

Some useful three-point formulas

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

Three-Point Formulas (1/3)

With $x_j = x_0, x_1 = x_0 + h$, and $x_2 = x_0 + 2h$, the general 3-point formula becomes

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

Some useful three-point formulas

$$f'(x_j) = f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right] + f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right]$$
$$+ f(x_2)\left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}\right] + \frac{1}{6}f^{(3)}(\xi_j)\prod_{\substack{k=0\\k\neq j}}^{2}(x_j - x_k)$$

Three-Point Formulas (2/3)

Doing the same for $x_j = x_1$ gives

$$f'(x_1) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_2)\right] - \frac{h^2}{6}f^{(3)}(\xi_1)$$

Some useful three-point formulas

$$f'(x_j) = f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right] + f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right] + f(x_2)\left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}\right] + \frac{1}{6}f^{(3)}(\xi_j)\prod_{\substack{k=0\\k\neq j}}^{2}(x_j - x_k)$$

Three-Point Formulas (3/3)

. . . and for $x_j = x_2$, we obtain

$$f'(x_2) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_1) + \frac{3}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_2)$$

Some useful three-point formulas

Three-Point Formulas: Further Simplification

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Three-Point Formulas: Further Simplification

Since $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, these formulas can also be expressed as

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

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

$$f'(x_0+2h) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_0+h) + \frac{3}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_2)$$

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

$$f'(x_0+2h) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_0+h) + \frac{3}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_2)$$

As a matter of convenience, the variable substitution x_0 for $x_0 + h$ is used in the middle equation to change this formula to an approximation for $f'(x_0)$. A similar change, x_0 for $x_0 + 2h$, is used in the last equation.

Some useful three-point formulas

Three-Point Formulas: Further Simplification (Cont'd)

This gives three formulas for approximating $f'(x_0)$:

Some useful three-point formulas

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$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

$$f'(x_0) = \frac{1}{2h}[-f(x_0-h) + f(x_0+h)] - \frac{h^2}{6}f^{(3)}(\xi_1), \quad \text{and}$$

$$f'(x_0) = \frac{1}{2h}[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)] + \frac{h^2}{3}f^{(3)}(\xi_2)$$

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This gives three formulas for approximating $f'(x_0)$:

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

$$f'(x_0) = \frac{1}{2h}[-f(x_0 - h) + f(x_0 + h)] - \frac{h^2}{6}f^{(3)}(\xi_1), \quad \text{and}$$

$$f'(x_0) = \frac{1}{2h}[f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0)] + \frac{h^2}{3}f^{(3)}(\xi_2)$$

Finally, note that the last of these equations can be obtained from the first by simply replacing h with $-h$, so there are actually only two formulas.

Some useful three-point formulas

Three-Point Endpoint Formula

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

where ξ_0 lies between x_0 and $x_0 + 2h$.

Some useful three-point formulas

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Three-Point Midpoint Formula

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

where ξ_1 lies between $x_0 - h$ and $x_0 + h$.

Some useful three-point formulas

$$(1) \quad f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

$$(2) \quad f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f^{(3)}(\xi_1)$$

Comments

Some useful three-point formulas

$$(1) \quad f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

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Comments

- Although the errors in both Eq. (1) and Eq. (2) are $O(h^2)$, the error in Eq. (2) is approximately half the error in Eq. (1).

Some useful three-point formulas

$$(1) \quad f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

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Comments

- Although the errors in both Eq. (1) and Eq. (2) are $O(h^2)$, the error in Eq. (2) is approximately half the error in Eq. (1).
- This is because Eq. (2) uses data on both sides of x_0 and Eq. (1) uses data on only one side.

Some useful three-point formulas

$$(1) \quad f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3}f^{(3)}(\xi_0)$$

$$(2) \quad f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f^{(3)}(\xi_1)$$

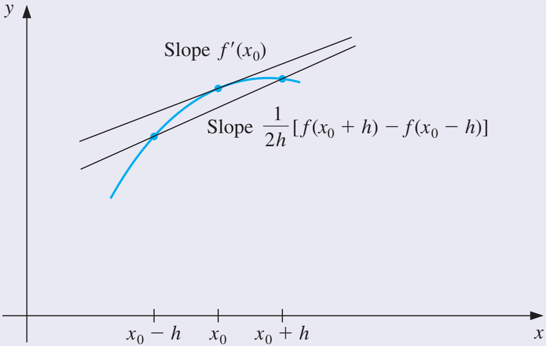
Comments

- Although the errors in both Eq. (1) and Eq. (2) are $O(h^2)$, the error in Eq. (2) is approximately half the error in Eq. (1).
- This is because Eq. (2) uses data on both sides of x_0 and Eq. (1) uses data on only one side.
- Note also that f needs to be evaluated at only two points in Eq. (2), whereas in Eq. (1) three evaluations are needed.

Three-Point Midpoint Formula

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

where ξ_1 lies between $x_0 - h$ and $x_0 + h$.



Examples of five-point formulas

Five-Point Midpoint Formula

$$f'(x_0) = \frac{1}{12h}[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30} f^{(5)}(\xi)$$

where ξ lies between $x_0 - 2h$ and $x_0 + 2h$.

Examples of five-point formulas

Five-Point Midpoint Formula

$$f'(x_0) = \frac{1}{12h}[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30} f^{(5)}(\xi)$$

where ξ lies between $x_0 - 2h$ and $x_0 + 2h$.

Five-Point Endpoint Formula

$$f'(x_0) = \frac{1}{12h}[-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h)] + \frac{h^4}{5} f^{(5)}(\xi)$$

where ξ lies between x_0 and $x_0 + 4h$.

Questions?

Reference Material

The Lagrange Polynomial: Theoretical Error Bound

Suppose $x_0, x_1, \ldots, x_n$ are distinct numbers in the interval $[a, b]$ and $f \in C^{n+1}[a, b]$. Then, for each x in $[a, b]$, a number $\xi(x)$ (generally unknown) between $x_0, x_1, \ldots, x_n$, and hence in (a, b), exists with

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

where $P(x)$ is the interpolating polynomial given by

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

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