Numerical Analysis

(ENME 602)

Spring 2021

Lecture 8

Dr. Hesham H. Ibrahim
Associate Professor, Mechatronics Department.
hesham.hamed-ahmed@guc.edu.eg
Office C7.04

Lecture 8

Numerical Differentiation

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

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

8.1 Introduction to Numerical Differentiation

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Approximating a Derivative

- The derivative of the function f at x_0 is

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

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

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

  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.

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 $x_1 \in [a, b]$.
- 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.

8.1 Introduction to 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

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

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

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

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

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

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

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

8.1 Introduction to Numerical Differentiation

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

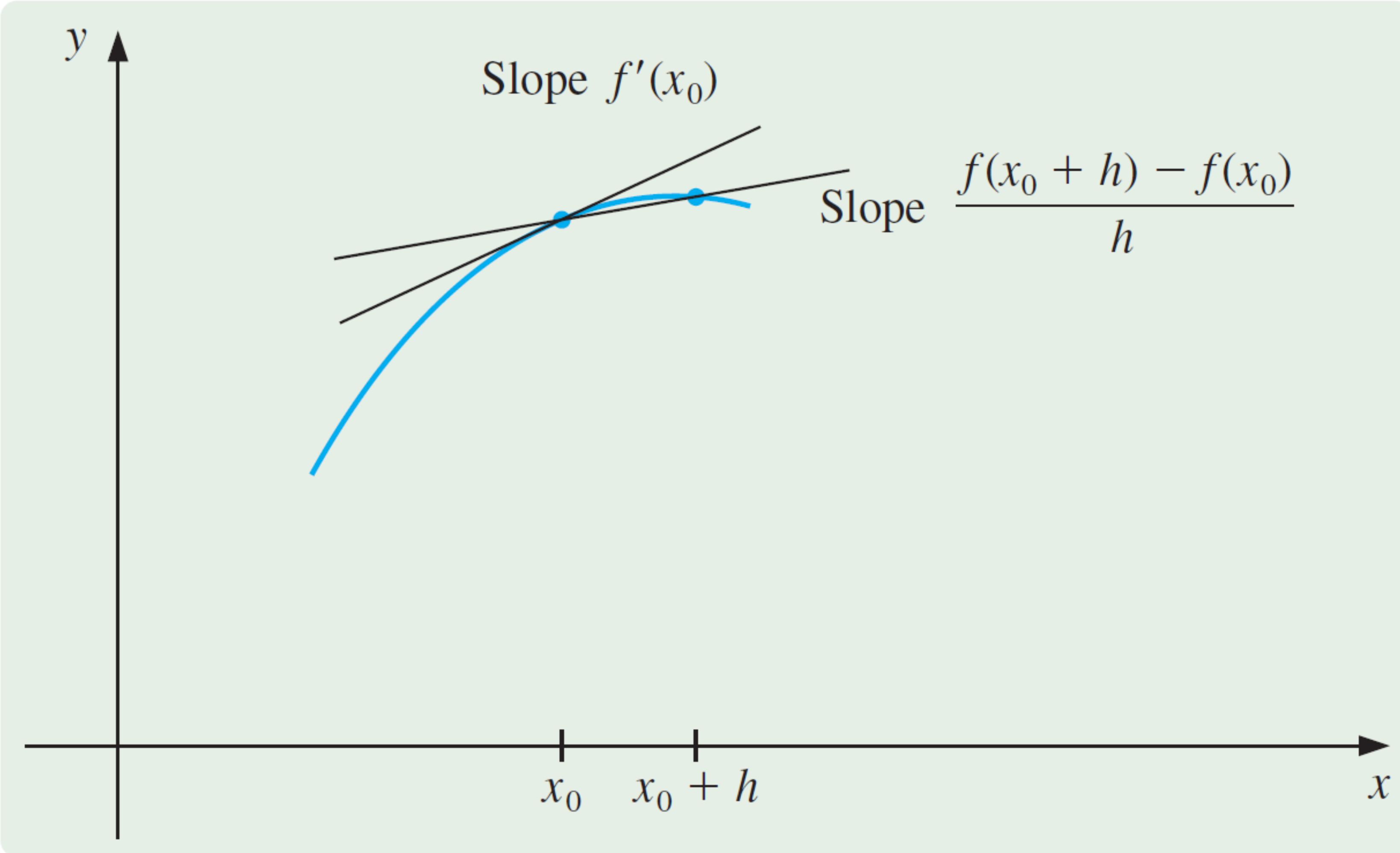
Forward-Difference and Backward-Difference Formulae

- 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 $x_0 + h$.
- This formula is known as the forward-difference formula if $h > 0$ and the backward-difference formula if $h < 0$.

8.1 Introduction to Numerical Differentiation



8.1 Introduction to 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.

Solution (1/3)

The forward-difference formula

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

with $h = 0.1$ gives

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

8.1 Introduction to Numerical Differentiation

Solution (2/3)

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

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

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.

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.

8.2 General Derivative Approximation Formulas

8.2 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 $x_0, x_1, \ldots, x_n$.

8.2 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

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

8.2 General Derivative Approximation Formulas

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

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

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

which is called an $(n+1)$-point formula to approximate $f'(x_j)$.

8.2 General Derivative Approximation Formulas

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

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

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

8.3 Three-point Formulas

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Important Building Blocks

Since

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

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

$$\begin{aligned} L_1'(x) &= \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \\ L_2'(x) &= \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} \end{aligned}$$

8.3 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

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

becomes for $n = 2$:

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

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

8.3 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

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

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

8.3 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 (1/3)

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

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

8.3 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 (2/3)

Doing the same for $x_j = x_1$ gives

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

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

Three-Point Formulas (3/3)

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

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

8.3 Three-point Formulas

Three-Point Formulas: Further Simplification

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

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

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

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

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.

8.3 Three-point Formulas

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

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.

8.3 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 $x_0 + 2h$.

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 $x_0 + h$.

8.3 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

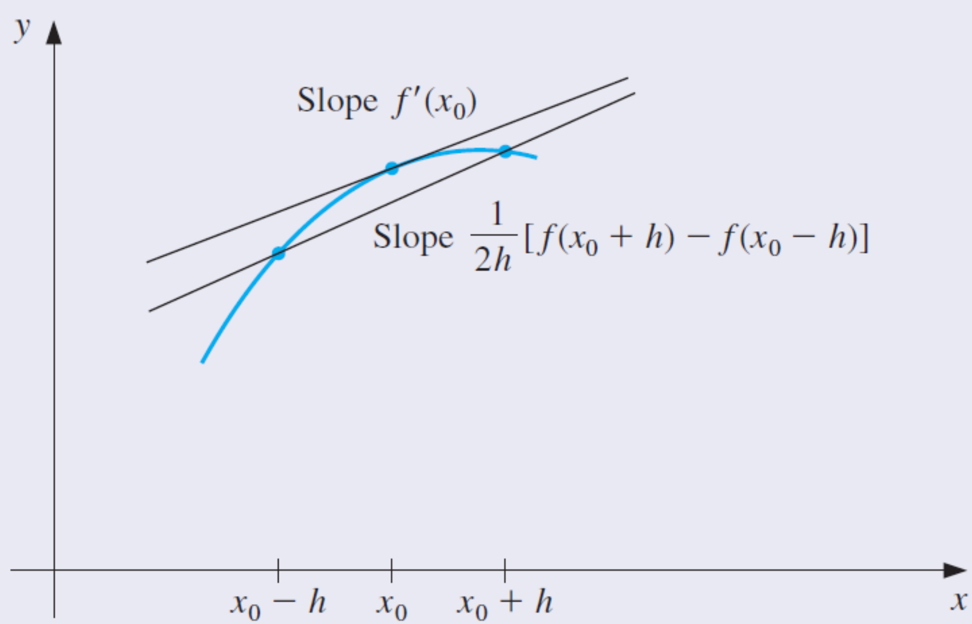
- Although the errors in both Eq. (1) and Eq. (2) are $O(h^2)$, the error in Eq. (2) is approximately half the error in Eq. (1).
- This is because Eq. (2) uses data on both sides of x_0 and Eq. (1) uses data on only one side.
- Note also that f needs to be evaluated at only two points in Eq. (2), whereas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

8.3 Three-point Formulas

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 $x_0 + h$.



8.4 Five-point Formulas

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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 $x_0 + 4h$.

8.5Application of the 3-Point and 5-Point Formulae

8.5 Application of the 3-Point and 5-Point Formulae

Example

Values for $f(x) = xe^x$ are given in the following table:

x	1.8	1.9	2.0	2.1	2.2
$f(x)$	10.889365	12.703199	14.778112	17.148957	19.855030

Use all the applicable three-point and five-point formulas to approximate $f'(2.0)$.

Solution (1/4)

- The data in the table permit us to find four different three-point approximations. ▸ See 3-Point Endpoint & Midpoint Formulae
- We can use the endpoint formula with $h = 0.1$ or with $h = -0.1$, and
- we can use the midpoint formula with $h = 0.1$ or with $h = 0.2$.

Solution (2/4)

Using the 3-point endpoint formula with $h = 0.1$ gives

$$\begin{aligned}
& \frac{1}{0.2}[-3f(2.0) + 4f(2.1) - f(2.2] \\
= \quad & 5[-3(14.778112) + 4(17.148957) - 19.855030)] = 22.032310
\end{aligned}$$

and with $h = -0.1$ gives 22.054525.

Using the 3-point midpoint formula with $h = 0.1$ gives

$$\frac{1}{0.2}[f(2.1) - f(1.9] = 5(17.148957 - 12.7703199) = 22.228790$$

and with $h = 0.2$ gives 22.414163.

Solution (3/4)

The only five-point formula for which the table gives sufficient data is the midpoint formula ▸ See Formula with $h = 0.1$. This gives

$$\begin{aligned}
&\frac{1}{1.2}[f(1.8) - 8f(1.9) + 8f(2.1) - f(2.2)] \\
=&\frac{1}{1.2}[10.889365 - 8(12.703199) + 8(17.148957) - 19.855030] \\
=&22.166999
\end{aligned}$$

If we had no other information, we would accept the five-point midpoint approximation using $h = 0.1$ as the most accurate, and expect the true value to be between that approximation and the three-point mid-point approximation, that is in the interval $[22.166, 22.229]$.

Solution (4/4)

The true value in this case is $f'(2.0) = (2+1)e^2 = 22.167168$, so the approximation errors are actually:

Method	h	Approximation Error
Three-point endpoint	0.1	1.35×10^{-1}
Three-point endpoint	-0.1	1.13×10^{-1}
Three-point midpoint	0.2	-2.47×10^{-1}
Three-point midpoint	0.1	-6.16×10^{-2}
Five-point midpoint	0.1	1.69×10^{-4}

8.6 Numerical Approximations to Higher Derivatives

8.6 Numerical Approximations to Higher Derivatives

Illustrative Method of Construction

Expand a function f in a third Taylor polynomial about a point x_0 and evaluate at $x_0 + h$ and $x_0 - h$. Then

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_1)h^4$$

and

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_{-1})h^4$$

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

8.6 Numerical Approximations to Higher Derivatives

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

Illustrative Method of Construction (Cont'd)

If we add these equations, the terms involving $f'(x_0)$ and $-f'(x_0)$ cancel, so

$$f(x_0+h) + f(x_0-h) = 2f(x_0) + f''(x_0)h^2 + \frac{1}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]h^4$$

Solving this equation for $f''(x_0)$ gives

$$f''(x_0) = \frac{1}{h^2}[f(x_0-h) - 2f(x_0) + f(x_0+h)] - \frac{h^2}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]$$

8.6 Numerical Approximations to Higher Derivatives

$$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]$$

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 $x_0 - h < \xi < x_0 + h$.

Note: If $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$, then it is also bounded, and the approximation is $O(h^2)$.

8.6 Numerical Approximations to Higher Derivatives

Example (Second Derivative Midpoint Formula)

Values for $f(x) = xe^x$ are given in the following table:

x	1.8	1.9	2.0	2.1	2.2
$f(x)$	10.889365	12.703199	14.778112	17.148957	19.855030

Use the second derivative midpoint formula ▸ Formula approximate $f'(2.0)$.

8.6 Numerical Approximations to Higher Derivatives

Example (Second Derivative Midpoint Formula): Cont'd

The data permits us to determine two approximations for $f''(2.0)$. Using the formula with $h = 0.1$ gives

$$\begin{aligned} & \frac{1}{0.01}[f(1.9) - 2f(2.0) + f(2.1)] \\ = \quad & 100[12.703199 - 2(14.778112) + 17.148957] = 29.593200 \end{aligned}$$

and using the formula with $h = 0.2$ gives

$$\begin{aligned} & \frac{1}{0.04}[f(1.8) - 2f(2.0) + f(2.2)] \\ = \quad & 25[10.889365 - 2(14.778112) + 19.855030] = 29.704275 \end{aligned}$$

The exact value is $f''(2.0) = 29.556224$. Hence the actual errors are -3.70×10^{-2} and -1.48×10^{-1}, respectively.

8.7 Round-Off Error Instability

8.7 Round-Off Error Instability

Concept of Total Error

- It is particularly important to pay attention to round-off error when approximating derivatives.
- To illustrate the situation, let us examine the three-point midpoint formula:

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

  more closely.
- Suppose that in evaluating $f(x_0+h)$ and $f(x_0-h)$ we encounter round-off errors $e(x_0+h)$ and $e(x_0-h)$.

8.7 Round-Off Error Instability

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

Concept of Total Error (Cont'd)

- Then our computations actually use the values $\tilde{f}(x_0+h)$ and $\tilde{f}(x_0-h)$, which are related to the true values $f(x_0+h)$ and $f(x_0-h)$ by

$$f(x_0+h) = \tilde{f}(x_0+h) + e(x_0+h) \quad \text{and} \quad f(x_0-h) = \tilde{f}(x_0-h) + e(x_0-h)$$

- The total error in the approximation,

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

is due both to round-off error, the first part, and to truncation error.

8.7 Round-Off Error Instability

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

Concept of Total Error (Cont'd)

If we assume that the round-off errors $e(x_0 \pm h)$ are bounded by some number $\varepsilon > 0$ and that the third derivative of f is bounded by a number $M > 0$, then

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| \leq \frac{\varepsilon}{h} + \frac{h^2}{6} M$$

8.7 Round-Off Error Instability

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| \le \frac{\varepsilon}{h} + \frac{h^2}{6}M$$

Concept of Total Error (Cont'd)

- To reduce the truncation error, $h^2M/6$, we need to reduce h.
- But as h is reduced, the round-off error ε/h grows.
- In practice, then, it is seldom advantageous to let h be too small because, in that case, the round-off error will dominate the calculations.

8.7 Round-Off Error Instability

Example

Consider using the values in the following table

x	$\sin x$	x	$\sin x$
0.800	0.71736	0.901	0.78395
0.850	0.75128	0.902	0.78457
0.880	0.77074	0.905	0.78643
0.890	0.77707	0.910	0.78950
0.895	0.78021	0.920	0.79560
0.898	0.78208	0.950	0.81342
0.899	0.78270	1.000	0.84147

to approximate $f'(0.900)$, where $f(x) = \sin x$. The true value is $\cos 0.900 = 0.62161$.

8.7 Round-Off Error Instability

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| \le \frac{\varepsilon}{h} + \frac{h^2}{6}M$$

Solution (1/4)

The formula

$$f'(0.900) \approx \frac{f(0.900+h) - f(0.900-h)}{2h}$$

with different values of h, gives the approximations in the following table.

8.7 Round-Off Error Instability

Solution (2/4)

h	Approximation to $f'(0.900)$	Error
0.001	0.62500	0.00339
0.002	0.62250	0.00089
0.005	0.62200	0.00039
0.010	0.62150	-0.00011
0.020	0.62150	-0.00011
0.050	0.62140	-0.00021
0.100	0.62055	-0.00106

The optimal choice for h appears to lie between 0.005 and 0.05.

8.7 Round-Off Error Instability

Solution (3/4)

We can use calculus to verify that a minimum for

$$e(h) = \frac{\varepsilon}{h} + \frac{h^2}{6}M,$$

occurs at $h = \sqrt[3]{3\varepsilon/M}$, where

$$M = \max_{x\in[0.800,1.00]} |f'''(x)| = \max_{x\in[0.800,1.00]} |\cos x| = \cos 0.8 \approx 0.69671.$$

Because values of f are given to five decimal places, we will assume that the round-off error is bounded by $\varepsilon = 5 \times 10^{-6}$.

8.7 Round-Off Error Instability

Solution (4/4)

Therefore, the optimal choice of h is approximately

$$h = \sqrt[3]{3\varepsilon/M} = \sqrt[3]{\frac{3(0.000005)}{0.69671}} \approx 0.028,$$

which is consistent with the results in the earlier table.

- In practice, we cannot compute an optimal h to use in approximating the derivative, since we have no knowledge of the third derivative of the function.
- But we must remain aware that reducing the step size will not always improve the approximation.

Thank You

"Numerical Integration"