Numerical Differentiation & Integration

Numerical Differentiation II

Numerical Analysis (9th Edition)

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Beamer Presentation Slides
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Outline

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1. Application of the 3-Point and 5-Point Formulae

2. Numerical Approximations to Higher Derivatives

Outline

Numerical Differentiation: Application of the 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 $f'(2.0)$.

Numerical Differentiation: Application of the Formulae

Solution (1/4)

- The data in the table permit us to find four different three-point approximations. ▸ See 3-Point Endpoint & Midpoint Formulae

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- 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 $h = 0.2$.

Numerical Differentiation: Application of the Formulae

Solution (2/4)

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

$$\frac{1}{0.2}[-3f(2.0) + 4f(2.1) - f(2.2)]$$

Numerical Differentiation: Application of the Formulae

Solution (2/4)

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

Numerical Differentiation: Application of the Formulae

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

and with $h = -0.1$ gives 22.054525.

Numerical Differentiation: Application of the Formulae

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

$$\frac{1}{0.2}[f(2.1) - f(1.9)]$$

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

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

Numerical Differentiation: Application of the Formulae

Solution (2/4)

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

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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.

Numerical Differentiation: Application of the Formulae

Solution (3/4)

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

Numerical Differentiation: Application of the Formulae

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

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

Numerical Differentiation: Application of the Formulae

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

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

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 $[22.166, 22.229]$.

Numerical Differentiation: Application of the Formulae

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}

Outline

Numerical Approximations to Higher Derivatives

Illustrative Method of Construction

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

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

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

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}
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Illustrative Method of Construction (Cont'd)

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

Numerical Approximations to Higher Derivatives

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Illustrative Method of Construction (Cont'd)

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

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

Numerical Approximations to Higher Derivatives

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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

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

Numerical Approximations to Higher Derivatives

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

Illustrative Method of Construction (Cont'd)

Suppose $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$. Since $\frac{1}{2}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]$ is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_{-1})$, the Intermediate Value Theorem ▸ Theorem implies that a number ξ exists between ξ_1 and ξ_{-1}, and hence in $(x_0 - h, x_0 + h)$, with

$$f^{(4)}(\xi) = \frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]$$

Numerical Approximations to Higher Derivatives

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Suppose $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$. Since $\frac{1}{2}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]$ is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_{-1})$, the Intermediate Value Theorem ▸ Theorem implies that a number ξ exists between ξ_1 and ξ_{-1}, and hence in $(x_0 - h, x_0 + h)$, with

$$f^{(4)}(\xi) = \frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]$$

This permits us to rewrite the formula in its final form:

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

Numerical Approximations to Higher Derivatives

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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 $O(h^2)$.

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 $f'(2.0)$.

Numerical Approximations to Higher Derivatives

Example (Second Derivative Midpoint Formula): Cont'd

The data permits us to determine two approximations for $f''(2.0)$.

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

$$\frac{1}{0.01}[f(1.9) - 2f(2.0) + f(2.1)]$$

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

$$\frac{1}{0.01}[f(1.9) - 2f(2.0) + f(2.1)]$$

$$= 100[12.703199 - 2(14.778112) + 17.148957] = 29.593200$$

Numerical Approximations to Higher Derivatives

Example (Second Derivative Midpoint Formula): Cont'd

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and using the formula with $h = 0.2$ gives

$$\frac{1}{0.04}[f(1.8) - 2f(2.0) + f(2.2)]$$

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

$$\frac{1}{0.01}[f(1.9) - 2f(2.0) + f(2.1)]$$

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and using the formula with $h = 0.2$ gives

$$\frac{1}{0.04}[f(1.8) - 2f(2.0) + f(2.2)]$$

$$= 25[10.889365 - 2(14.778112) + 19.855030] = 29.704275$$

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

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

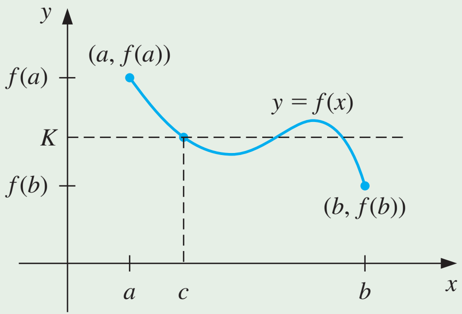
The exact value is $f''(2.0) = 29.556224$. Hence the actual errors are -3.70×10^{-2} and -1.48×10^{-1}, respectively.

Questions?

Reference Material

Intermediate Value Theorem

If $f \in C[a,b]$ and K is any number between $f(a)$ and $f(b)$, then there exists a number $c \in (a,b)$ for which $f(c) = K$.



(The diagram shows one of 3 possibilities for this function and interval.)

Return to Numerical Approximations to Higher Derivatives

Numerical Differentiation Formulae

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 $x_0 + h$.

Return to 3-Point Calculations

Numerical Differentiation Formulae

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 $x_0 + 4h$.

Return to 5-Point Calculations

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 Example on the Second Derivative Midpoint Formula