Numerical Analysis

Lecture 10: Numerical Differentiation

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Outline

1. Numerical Differentiation
2. General Derivative Approximation Formulas
3. Three-point Derivative Approximation Formulas
4. Numerical Approximations to Higher Derivatives
5. Round-Off Error Instability
6. Richardson's Extrapolation

Introduction to Numerical Differentiation

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.

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

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

for some $\xi(x)$ between x_0 and x_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

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

Introduction to 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

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

Introduction to Numerical Differentiation

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

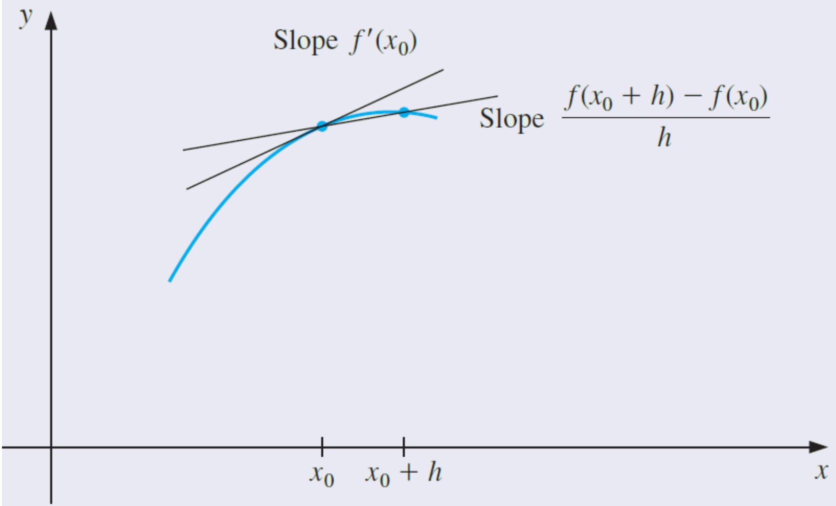
Forward-Difference and Backward-Difference Formulate

- 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 $h < 0$.

Introduction to Numerical Differentiation



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.

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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

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

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)

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

Outline

General Derivative Approximation Formulas

Method of Construction

- To obtain general derivative approximation formulas, suppose that $\{x_0, x_1, \cdots, x_n\}$ are $(n+1)$ distinct numbers in some interval I and that $f \in C^{n+1}(I)$.
- From the interpolation error 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 denotes the kth Lagrange coefficient polynomial for f at $x_0, x_1, \cdots, x_n$.

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

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

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

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

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

General Derivative Approximation Formulas

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

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.

Outline

Three-point Formulas

Important Building Blocks

Since

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

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

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

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

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

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

becomes for $n = 2$:

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

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

Three-point Formulas

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

Assumption

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

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

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

Three-point Formulas

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

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

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

Three-point Formulas

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

Three-Point Formulas (2/3)

Doing the same for $x_j = x_1$ gives

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

Three-point Formulas

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

Three-Point Formulas (3/3)

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

$$f'(x_2) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_1) + \frac{3}{2}f(x_2)\right] + \frac{h^2}{6}f^{(3)}(\xi_2)$$

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.

Three-point Formulas

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

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

$$
\begin{aligned}
f'(x_0) &= \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0) \\
f'(x_0) &= \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1) \\
f'(x_0) &= \frac{1}{2h}\left[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)\right] + \frac{h^2}{3} f^{(3)}(\xi_2)
\end{aligned}
$$

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.

Three-point Formulas

Three-Point Endpoint Formula

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

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

Three-Point Midpoint Formula

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

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

Three-point Formulas

$$
\begin{aligned}
(1)\quad f'(x_0) &= \frac{1}{2h}\left[-3f(x_0)+4f(x_0+h)-f(x_0+2h)\right]+\frac{h^2}{3}f^{(3)}(\xi_0)\\
(2)\quad f'(x_0) &= \frac{1}{2h}\left[f(x_0+h)-f(x_0-h)\right]-\frac{h^2}{6}f^{(3)}(\xi_1)
\end{aligned}
$$

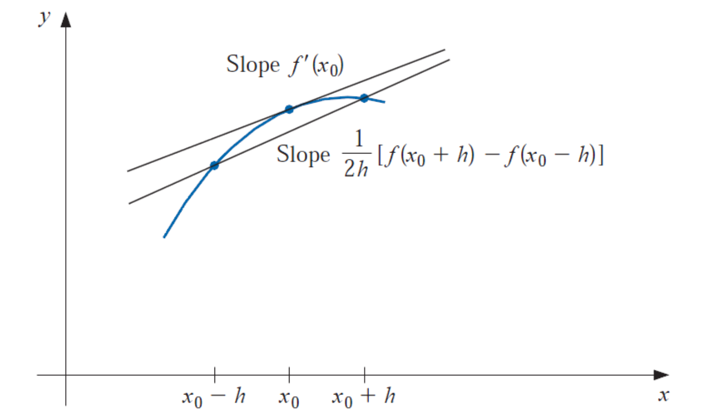
Comments

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

Three-point Formulas

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

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



Five-Point Formulas

Five-Point Endpoint Formula

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

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

Five-Point Midpoint Formula

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

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

Three-Point vs. Five-Point

Example

Three-Point and Five-Point formulas to approximate $f(x) = xe^x$ at $x = 2.0$.

- Three-point endpoint with $h = 0.1$: 1.35×10^{-1}
- Three-point endpoint with $h = -0.1$: 1.13×10^{-1}
- Three-point midpoint with $h = 0.1$: -6.16×10^{-2}
- Three-point midpoint with $h = 0.2$: -2.47×10^{-1}
- Five-point midpoint with $h = 0.1$: 1.69×10^{-4}

Outline

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

Numerical Approximations to Higher Derivatives

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

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

Illustrative Method of Construction (Cont'd)

Adding these equations, the terms involving $f'(x_0)$ cancel

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

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

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

Numerical Approximations to Higher Derivatives

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

Illustrative Method of Construction (Cont'd)

Suppose $f^{(4)}$ is continuous on $[x_0-h,x_0+h]$. Since $\frac{1}{2}\left[f^{(4)}(\xi_1)+f^{(4)}(\xi_{-1})\right]$ is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_{-1})$, the Intermediate Value 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

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

Second Derivative Midpoint Formula

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

for some $\xi \in [x_0 - h, x_0 + h]$.

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

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 approximate $f''(2.0)$.

Numerical Approximations to Higher Derivatives

Example

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

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

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

and using the formula with $h = 0.2$ gives

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

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

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

Outline

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:

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

  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 $e(x_0-h)$.

Round-Off Error Instability

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

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

- 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.

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 error $e(x_0 \pm h)$ are bounded by some number $\epsilon > 0$ and that the third derivative of f is bounded by a number $M > 0$, then

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

Round-Off Error Instability

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

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.

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 $\cos 0.900 = 0.62161$.

Round-Off Error Instability

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

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.

Round-Off Error Instability

Solution (3/4)

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.

Round-Off Error Instability

Solution (3/4)

We can use calculus to verify that a minimum for

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

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

$$M = \max_{x \in [0.800, 1.000]} |f'''(x)| = \max_{x \in [0.800, 1.000]} |\cos x| = \cos\ 0.8 \approx 0.69671.$$

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

Round-Off Error Instability

Solution (4/4)

Therefore, the optimal choice of h is approximately

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

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.

Round-Off Error Instability

Concluding Remarks

- We have considered only the round-off error problems that are presented by the three-point midpoint formula, but similar difficulties occur with all the differentiation formulas.
- The reason can be traced to the need to divide by a power of h.
- Division by small numbers tends to exaggerate round-off error, and this operation should be avoided if possible.
- In the case of numerical differentiation, we cannot avoid the problem entirely, although the higher-order methods reduce the difficulty.

Round-Off Error Instability

Concluding Remarks

- As approximation methods, numerical differentiation is unstable, since the small values of h needed to reduce truncation error also cause the round-off error to grow.
- This is the first class of unstable methods we have encountered, and these techniques would be avoided if it were possible.
- However, in addition to being used for computational purposes, the formulas are needed for approximating the solutions of ordinary and partial-differential equations.

Outline

Richardson's Extrapolation

Generating the Extrapolation Formula

- To see specifically how we can generate the extrapolation formulas, consider the $O(h)$ formula for approximating M

$$M = N_1(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots$$

- The formula is assumed to hold for all positive h, so we replace the parameter h by half its value.
- Then we have a second $O(h)$ approximation formula

$$M = N_1(\frac{h}{2}) + K_1 \frac{h}{2} + K_2 \frac{h^2}{4} + K_3 \frac{h^3}{8} + \cdots$$

Richardson's Extrapolation

$$M = N_1(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots$$

$$M = N_1(\frac{h}{2}) + K_1 \frac{h}{2} + K_2 \frac{h^2}{4} + K_3 \frac{h^3}{8} + \cdots$$

Generating the Extrapolation Formula (Cont'd)

Subtracting the first from twice the second eliminates the term involving K_1 and gives

$$M = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right] - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots$$

Richardson's Extrapolation

$$M = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right] - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots$$

Generating the Extrapolation Formula (Cont'd)

- Define

$$N_2(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right]$$

- Then the above equation is an $O(h^2)$ approximation formula for M:

$$M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots$$

Richardson's Extrapolation

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

- In an earlier example, we used the forward-difference method

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

  with $h = 0.1$ and $h = 0.05$ to find approximations to $f'(1.8)$ for $f(x) = \ln x$.
- Assume that this formula has truncation error $O(h)$ and use extrapolation on these values to see if this results in a better approximation.

Richardson's Extrapolation

Solution

Using the forward-difference method

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

we find that

$$\begin{aligned} \text{with } \ h = 0.1: &\quad f'(1.8) \approx 0.5406722 \\ \text{with } \ h = 0.05: &\quad f'(1.8) \approx 0.5479795 \end{aligned}$$

This implies that

$$N_1(0.1) = 0.5406722 \qquad \text{and} \qquad N_1(0.05) = 0.5479795$$

Richardson's Extrapolation

$$N_2(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right]$$

Solution

- Extrapolating these results gives the new approximation

$$\begin{aligned} N_2(0.1) &= N_1(0.05) + (N_1(0.05) - N_1(0.1)) \\ &= 0.5479795 + (0.5479795 - 0.5406722) \\ &= 0.555287 \end{aligned}$$

- The $h = 0.1$ and $h = 0.05$ results were found to be accurate to within 1.5×10^{-2} and 7.7×10^{-3}, respectively.
- Because $f'(1.8) = 1/1.8 = 0.\bar{5}$, the extrapolated value is accurate to within 2.7×10^{-4}.

Richardson's Extrapolation

When can be extrapolation applied?

Extrapolation can be applied whenever the truncation error for a formula has 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 $\alpha_1 < \alpha_2 < \cdots < \alpha_m$.

Richardson's Extrapolation

More accuracy

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
1: $N_1(h)$			
2: $N_1(\frac{h}{2})$	**3:** $N_2(h)$		
4: $N_1(\frac{h}{4})$	**5:** $N_2(\frac{h}{2})$	**6:** $N_3(h)$	
7: $N_1(\frac{h}{8})$	**8:** $N_2(\frac{h}{4})$	**9:** $N_3(\frac{h}{2})$	**10:** $N_4(h)$

Richardson's Extrapolation

Ensuring accuracy

- Each column beyond the first in the extrapolation table is obtained by a simple averaging process, so the technique can produce high-order approximations with minimal computational cost.
- However, as k increases, the round-off error in $N_1(h/2^k)$ will generally increase because the instability of numerical differentiation is related to the step size of $h/2^k$.
- Also, the higher-order formulas depending increasingly on the entry to their immediate left in the table, which is the reason we recommend comparing the final diagonal entries to ensure accuracy.

Assignment

Assignment

- Reading assignment: Chap 4.1-4.2