CSER 2207: Numerical Analysis

Lecture-13
Numerical Differentiation

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Higher Order Derivatives

Methods can also be derived to find approximations to higher derivatives of a functic using only tabulated values of the function at various points. The derivation is algebraical tedious, however, so only a representative procedure will be presented.

Expand a function f in a third Taylor polynomial about a point x_0 and evaluate at $x_0 +$ 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 $x_0 - h < \xi_{-1} < x_0 < \xi_1 < x_0 + h$.

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

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

Second Derivative

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

$$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]. \qquad (4.8)$$

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 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 Eq. (4.8) in its final form.

Second Derivative Midpoint Formula

- $$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12}f^{(4)}(\xi), \qquad (4.9)$$

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

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

Example

Example 3 In Example 2 we used the data shown in Table 4.3 to approximate the first derivative of $f(x) = xe^x$ at $x = 2.0$. Use the second derivative formula (4.9) to approximate $f''(2.0)$.

Table 4.3

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

Solution The data permits us to determine two approximations for $f''(2.0)$. Using (4.9) with $h = 0.1$ gives

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

and using (4.9) with $h = 0.2$ gives

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

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

Richardson’s Extrapolation

- **Given**: A formula $N_1(h)$ that approximates an unknown constant M for any $h \neq 0$.
- **Given**: Truncation error satisfies power series for $h \neq 0$

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots = O(h), \qquad (1)$$

with (unknown) constants $K1, K_2, K_3, \cdots$.

$$\boxed{\text{Goal: Generate higher order approximations}}$$

- **Key**: Equation (1) works for *any* $h \neq 0$.

Extrapolation, Step 1

$$
\begin{aligned}
M - N_1(h) &= K_1 h + K_2 h^2 + K_3 h^3 + \cdots \,, & (2) \\
M - N_1(\frac{h}{2}) &= K_1(\frac{h}{2}) + K_2(\frac{h}{2})^2 + K_3(\frac{h}{2})^3 + \cdots \,. & (3)
\end{aligned}
$$

(3)$\times$2$-$ (2):

$$
\begin{aligned}
M - N_2(h) &= -\frac{K_2}{2} h^2 - \frac{3K_3}{4} h^3 - \cdots - (1 - 2^{-(t-1)}) K_t h^t - \cdots \,, \\
&\stackrel{def}{=} \widehat{K}_2 h^2 + \widehat{K}_3 h^3 + \cdots \widehat{K}_t h^t + \cdots = O\left(h^2\right) \,, \qquad (4)
\end{aligned}
$$

where $\quad N_2(h) = N_1(\frac{h}{2}) + \left(N_1(\frac{h}{2}) - N_1(h) \right) .$

$\boxed{\text{Equation (4) again power series, but now 2nd order.}}$

Extrapolation, Step 2

$$
\begin{aligned}
M - N_2(h) &= \widehat{K}_2 h^2 + \widehat{K}_3 h^3 + \cdots \widehat{K}_t h^t + \cdots\,, && (5) \\
M - N_2(\frac{h}{2}) &= \widehat{K}_2(\frac{h}{2})^2 + \widehat{K}_3(\frac{h}{2})^3 + + \cdots\,. && (6)
\end{aligned}
$$

$$\frac{(6)\times 2^2 - (5)}{2^2 - 1}:$$

$$M - N_3(h) = -\frac{\widehat{K}_3}{6} h^3 - \cdots - \frac{1 - 2^{-(t-2)}}{3} \widehat{K}_t h^t - \cdots\,,$$

$$\text{where} \quad N_3(h) \stackrel{def}{=} N_2(\frac{h}{2}) + \frac{N_2(\frac{h}{2}) - N_2(h)}{3}.$$

$$\boxed{\text{One more power series, but now 3rd order.}}$$

Extrapolation, Step 3

- Assume

$$M - N_j(h) = \widehat{K}_j h^j + \widehat{K}_{j+1} h^{j+1} + \cdots \widehat{K}_t h^t + \cdots ,$$

- replace h by $h/2$:

$$M - N_j(\frac{h}{2}) = \widehat{K}_j (\frac{h}{2})^j + \widehat{K}_{j+1} (\frac{h}{2})^{j+1} + \cdots \widehat{K}_t (\frac{h}{2})^t + \cdots .$$

$$\frac{\text{second equation } \times 2^j - \text{ first equation}}{2^j - 1}:$$

$$M - N_{j+1}(h) \quad = \quad -\frac{\widehat{K}_{j+1}}{2(2^j - 1)} h^{j+1} - \cdots = O\left(h^{j+1}\right),$$

$$\text{where} \quad N_{j+1}(h) \stackrel{def}{=} N_j(\frac{h}{2}) + \frac{N_j(\frac{h}{2}) - N_j(h)}{2^j - 1}.$$

Extrapolation Table

$$
\begin{array}{llll}
O(h) & O(h^2) & O(h^3) & O(h^4) \\
\hline
N_1(h) \searrow & & & \\
\quad\rightarrow & & & \\
N_1(\frac{h}{2}) \searrow & N_2(h) \searrow & & \\
\quad\rightarrow & \quad\rightarrow & & \\
N_1(\frac{h}{4}) \searrow & N_2(\frac{h}{2}) \searrow & N_3(h) \searrow & \\
N_1(\frac{h}{8}) \rightarrow & N_2(\frac{h}{4}) \rightarrow & N_3(\frac{h}{2}) \rightarrow & N_4(h)
\end{array}
$$

Example

In Example 1 of Section 4.1 we use the forward-difference method 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.

Solution In Example 1 of Section 4.1 we found that

$$\text{with } h = 0.1\text{: } f'(1.8) \approx 0.5406722, \quad \text{and} \quad \text{with } h = 0.05\text{: } f'(1.8) \approx 0.5479795.$$

This implies that

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

Extrapolating these results gives the new approximation

$$N_2(0.1) = N_1(0.05) + (N_1(0.05) - N_1(0.1)) = 0.5479795 + (0.5479795 - 0.5406722)$$
$$= 0.555287.$$

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 $f'(1.8) = 1/1.8 = 0.\overline{5}$, the extrapolated value is accurate to within 2.7×10^{-4}. ■

Thank You