CSC349A Numerical Analysis

Lecture 19

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2018

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Numerical Differentiation Formulas

- In Chapter 4, Taylor's Theorem is used to derive a numerical differentiation formula that was used to approximate a derivative in a mathematical model that was developed to determine the terminal velocity of a free-falling body (a parachutist).
- Recall Taylor's Theorem (with $n = 2$):

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \frac{f'''(\xi_1)}{3!}(x - x_0)^3$$

where ξ_1 lies between x and x_0.

Alternative Form of Taylor's Theorem

Taylor's Theorem can also be stated in terms of a step size, $h < 1$, by letting $h = x - x_0$ which implies that $x = x_0 + h$. Thus, Taylor's approxiamtion becomes

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

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

Forward Difference Approximation

Solving for $f'(x_0)$ in (1) gives

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

or

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0)}{h} \text{ with error } O(h).$$

Another Form of Taylor's Theorem

Consider yet another form of Taylor, where $x = x_0 - h$, thus $-h = x - x_0$ and

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{f''(x_0)}{2}h^2 - \frac{f'''(\xi_2)}{6}h^3 \qquad (2)$$

where ξ_2 lies between $x_0 - h$ and x_0.

Backward Difference Approximation

Solving for $f'(x_0)$ in (2) gives

$$\begin{aligned} f'(x_0)h =& f(x_0) - f(x_0 - h) + \frac{f''(x_0)}{2}h^2 - \frac{f'''(\xi_2)}{6}h^3 \\ f'(x_0) =& \frac{f(x_0) - f(x_0 - h)}{h} + \frac{f''(x_0)}{2}h - \frac{f'''(\xi_2)}{6}h^2 \end{aligned}$$

or

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h} \text{ with error } O(h).$$

Central Difference Approximation

A more accurate approximation to a first derivative can be obtained by taking a linear combination of these two Taylor Theorem approximations. Subtracting (2) from (1) gives

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0-h)}{2h} \text{ with error } O(h^2).$$

Example 1: Use forward and central difference approximations to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.25$$

at $x = 0.5$ using step size $h = 0.5$.

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High-Accuracy Differentiation Formulas

- Still more accurate approximations to $f'(x_0)$ can be obtained by taking linear combinations of more Taylor Theorem approximations and solving for $f'(x_0)$.
- FIGURES 23.1 to 23.3 on pages 656-657 in the text summarize other such formulas.

For example, Taylor Theorem approximations for each of

$$f(x_0 - 2h), f(x_0 - h), f(x_0 + 2h), f(x_0 + h)$$

can be used to derive the $O(h^4)$ approximation

$$f'(x_0) \approx \frac{1}{12h}\left[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)\right]$$

Example of Richardson's Extrapolation

- We can also use Richardson's Extrapolation to gain higher accuracy.

Example 1:

Use Richardson's extrapolation and the approximation formula

$$f'(x_0) \approx \frac{f(x_o + h) - f(x_0 - h)}{2h},$$

which has a truncation error of the form,

$$K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots ,$$

to approximate $f'(2)$ where $f(x) = xe^x$ and $h = 0.2$.

Final Solution of Example 1

The first 4 rows and columns of the Richardson's Extrapolation table are as follows:

	N_1	N_2	N_3	N_4
$h = 0.2$	22.4141607			
$h = 0.1$	22.2287869	22.1669956		
$h = 0.05$	22.1825649	22.1671575	22.1671683	
$h = 0.025$	22.1710169	22.1671676	22.1671683	22.1671683

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Numerical Differentiation Formulas for Higher Derivatives

Similar techniques can be applied to find formulas for higher derivatives. For example, we can derive $f''(x_0)$ by doing the following:

Example: Let $n = 3$ and use the following Taylor Approximations

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

and

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \frac{h^3}{6}f'''(x_0) + \frac{h^4}{24}f^{(4)}(\xi_2)$$

Numerical Differentiation Formula for $f''(x_0)$

Adding these gives:

$$f(x_0+h)+f(x_0-h) = 2f(x_0)+h^2 f''(x_0)+\frac{h^4}{24}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_2)\right]$$

and solving for the desired derivative $f''(x_0)$ gives

$$f''(x_0) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - \frac{h^2}{24}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_2)\right]$$

That is,

$$f''(x_0) \approx \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2}$$

with a truncation error of $O(h^2)$.