Numerical Differentiation & Integration

Numerical Differentiation III

Numerical Analysis (9th Edition)

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Outline

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Numerical Differentiation: Round-Off Error Instability

Concept of Total Error

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Numerical Differentiation: Round-Off Error Instability

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- To illustrate the situation, let us examine the three-point midpoint formula:

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

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Numerical Differentiation: Round-Off Error Instability

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

Numerical Differentiation: Round-Off Error Instability

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Concept of Total Error (Cont'd)

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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

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

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- 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.

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

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- 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.

Outline

Numerical Differentiation: 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 $\cos 0.900 = 0.62161$.

Numerical Differentiation: Round-Off Error Instability

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

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.

Numerical Differentiation: 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.

Numerical Differentiation: Round-Off Error Instability

Solution (3/4)

We can use calculus to verify that a minimum for

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

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

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Solution (4/4)

Therefore, the optimal choice of h is approximately

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

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- 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.

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- Division by small numbers tends to exaggerate round-off error, and this operation should be avoided if possible.

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- 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.

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Concluding Remarks (2/2)

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- This is the first class of unstable methods we have encountered, and these techniques would be avoided if it were possible.

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- 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.

Questions?