DTS104TC
NUMERICAL METHODS

LECTURE 7

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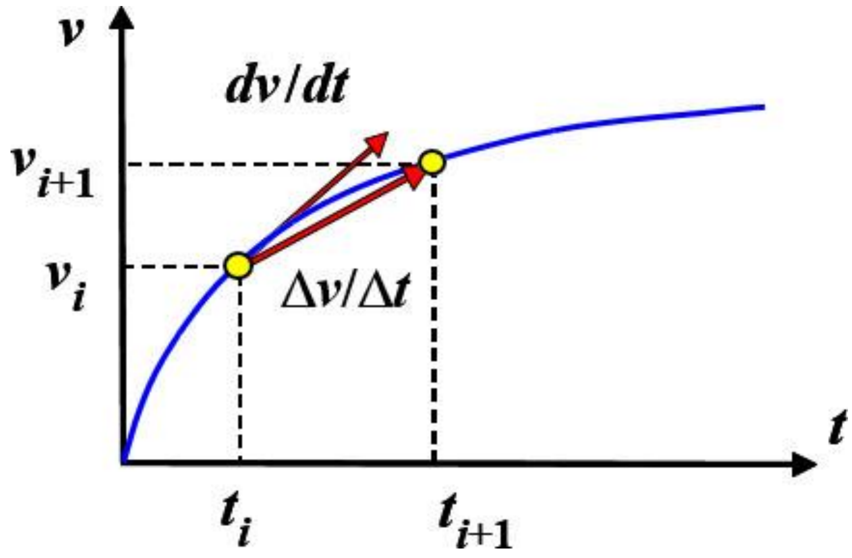
CONTENTS

- Truncation Errors
- Taylor Series
- Numerical Differentiation

TRUNCATION ERRORS

How we approximated the derivative



$$\frac{dv}{dt} \cong \frac{\Delta v}{\Delta t} = \frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i}$$

TRUNCATION ERRORS

$$\frac{dv}{dt} \cong \frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i}$$

Key questions:

Given $\Delta t = t_{i+1} - t_i$

How good is the approximation? Error.

What is benefit for reducing Δt? Convergence.

TAYLOR'S THEOREM

If a function f and its first $n + 1$ derivatives are continuous on an interval containing x_i and $x_{i+1} = x_i + h$, then the value of the function at x_{i+1} is given by

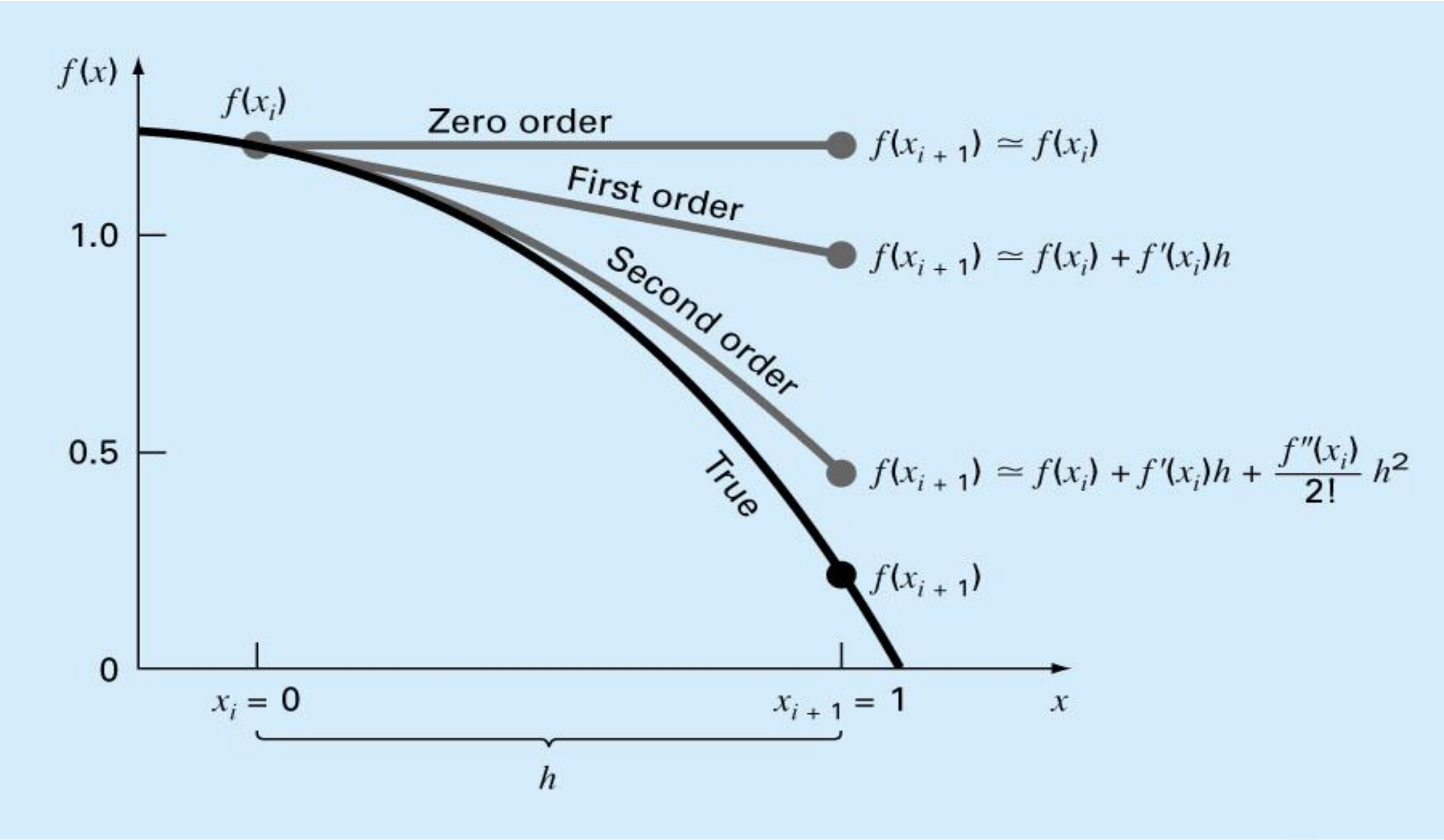
$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2$$

$$+\frac{f^{(3)}(x_i)}{3!}h^3 + \ldots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n$$

Where

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1}$$

TAYLOR SERIES



TRUNCATION ERRORS AND THE TAYLOR SERIES

- Non-elementary functions such as trigonometric, exponential, and others are expressed in an approximate fashion using Taylor series when their values, derivatives, and integrals are computed.
- Any smooth function can be approximated as a polynomial. Taylor series provides a means to predict the value of a function at one point in terms of the function value and its derivatives at another point.

TAYLOR SERIES EXAMPLE

To get the cos(x) for small x:

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots$$

If $x = 0.5$, the exact value is 0.877582562. The approximation is

$$\cos(0.5) = 1 - 0.125 + 0.0026041 - 0.0000127 + \ldots$$
$$= 0.877582465$$

From the supporting theory, for this series, the error is no greater than the first omitted term.

$$\therefore \quad \frac{x^8}{8!} \quad \text{for} \quad x = 0.5 \quad = 9.68812 \times 10^{-8}$$

The true error is $\left|0.877582562 - 0.877582465\right| = 9.66126 \times 10^{-8}$

THE TAYLOR SERIES REMAINDER

n^{th} order approximation

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''}{2!}(x_{i+1} - x_i)^2 + \dots$$
$$+ \frac{f^{(n)}}{n!}(x_{i+1} - x_i)^n + R_n$$

- define $h = (x_{i+1} - x_i)$ *step size*

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!} h^{(n+1)}$$

- Remainder term, R_n, accounts for all terms from $(n + 1)$ to infinity.

O(h) NOTATION

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2$$

$$+\frac{f^{(3)}(x_i)}{3!}h^3 + \ldots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n$$

where

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1}$$

Assumed to be
≈ constant

$$R_n = O(h^{n+1})$$

SUMMARY OF THE TAYLOR SERIES ERROR

- ξ is not known exactly, lies somewhere between $x_{i+1} > \xi > x_i$.
- Need to determine $f^{n+1}(x)$.
- To do this you need $f(x)$.
- If we knew $f(x)$, there wouldn't be any need to perform the Taylor series expansion!
- However, $R = O(h^{n+1})$, $(n+1)^{\text{th}}$ • order, the order of truncation error is h^{n+1}.
- $O(h)$, halving the step size will halve the error.
- $O(h^2)$, halving the step size will quarter the error.

TAYLOR SERIES ERROR

- Truncation error is decreased by addition of terms to the Taylor series.
- If h is sufficiently small, only a few terms may be required to obtain an approximation close enough to the actual value for practical purposes.

EXAMPLE:

- Estimating the truncation error of the velocity approximation of the derivative of the velocity

$$v(t_{i+1}) = v(t_i) + v'(t_i)\,(t_{i+1} - t_i) + \frac{v''(t_i)}{2!}(t_{i+1} - t_i)^2 + \ldots + R_n$$

$$v(t_{i+1}) = v(t_i) + v'(t_i)\,(t_{i+1} - t_i) + R_1$$

$$v'(t_i) = \underbrace{\frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i}}_{\text{First-order Approximation}} - \underbrace{\frac{R_1}{t_{i+1} - t_i}}_{\text{Truncation error}}$$

$$\frac{R_1}{t_{i+1} - t_i} = \frac{v''(\xi)}{2!}(t_{i+1} - t_i) = O(t_{i+1} - t_i) = O(h)$$

NUMERICAL DIFFERENTIATION

First forward divided difference:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} O(h)$$

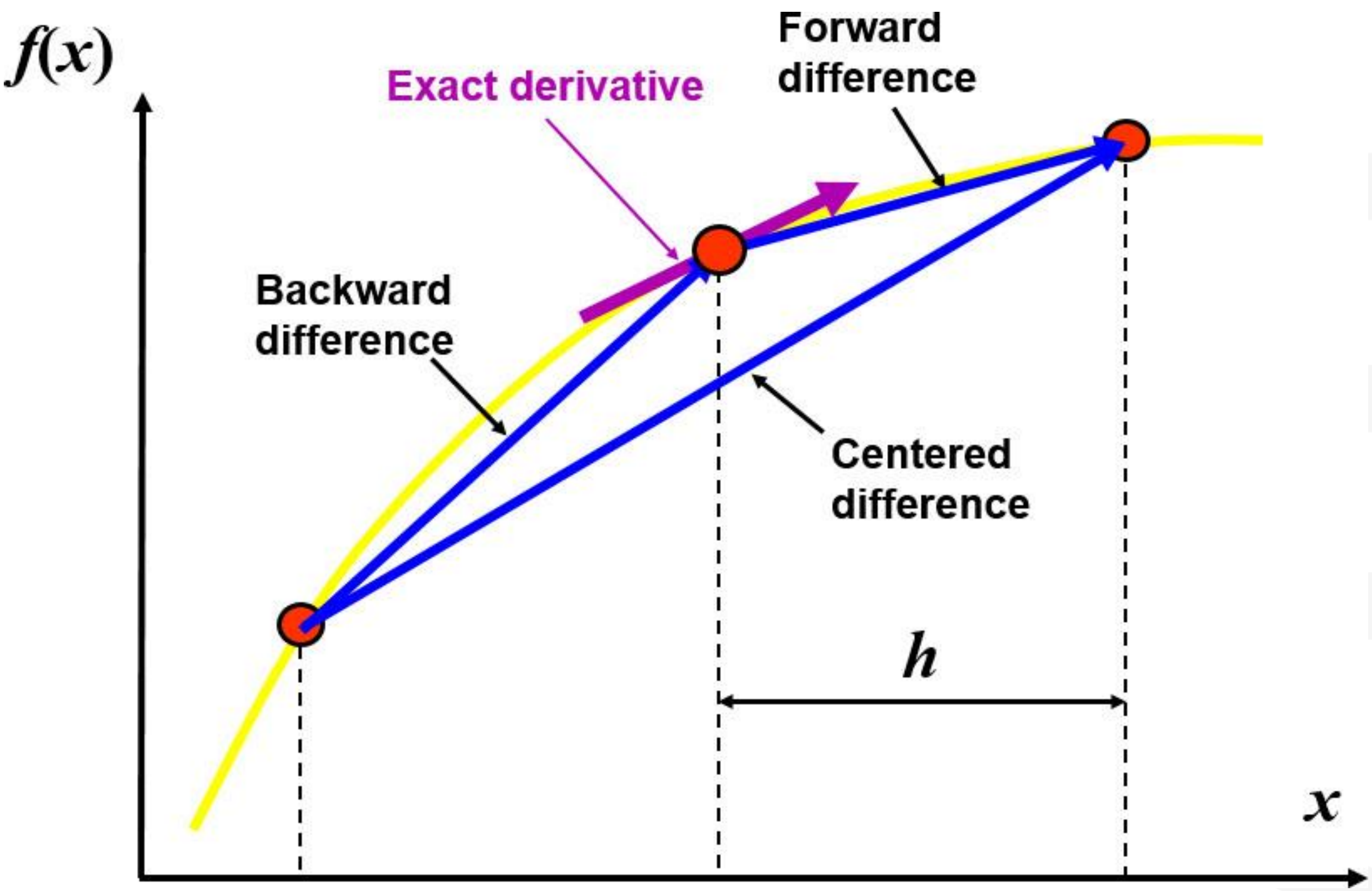
- *First backward divided difference:*

$$f'(x_i) \cong \frac{f(x_i) - f(x_{i-1})}{h} + O(h)$$

- *First centered divided difference:*

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2)$$

GRAPHICAL REPRESENTATION OF DIVIDED DIFFERENCES



CENTERED SECOND DIVIDED DIFFERENCE

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} + O(h^2)$$

- *By reformulating you can see it's the difference of two first derivative divided differences:*

$$f''(x_i) \cong \frac{\dfrac{f(x_{i+1}) - f(x_i)}{h} - \dfrac{f(x_i) - f(x_{i-1})}{h}}{h}$$

TWO-DIMENSIONAL TAYLOR SERIES

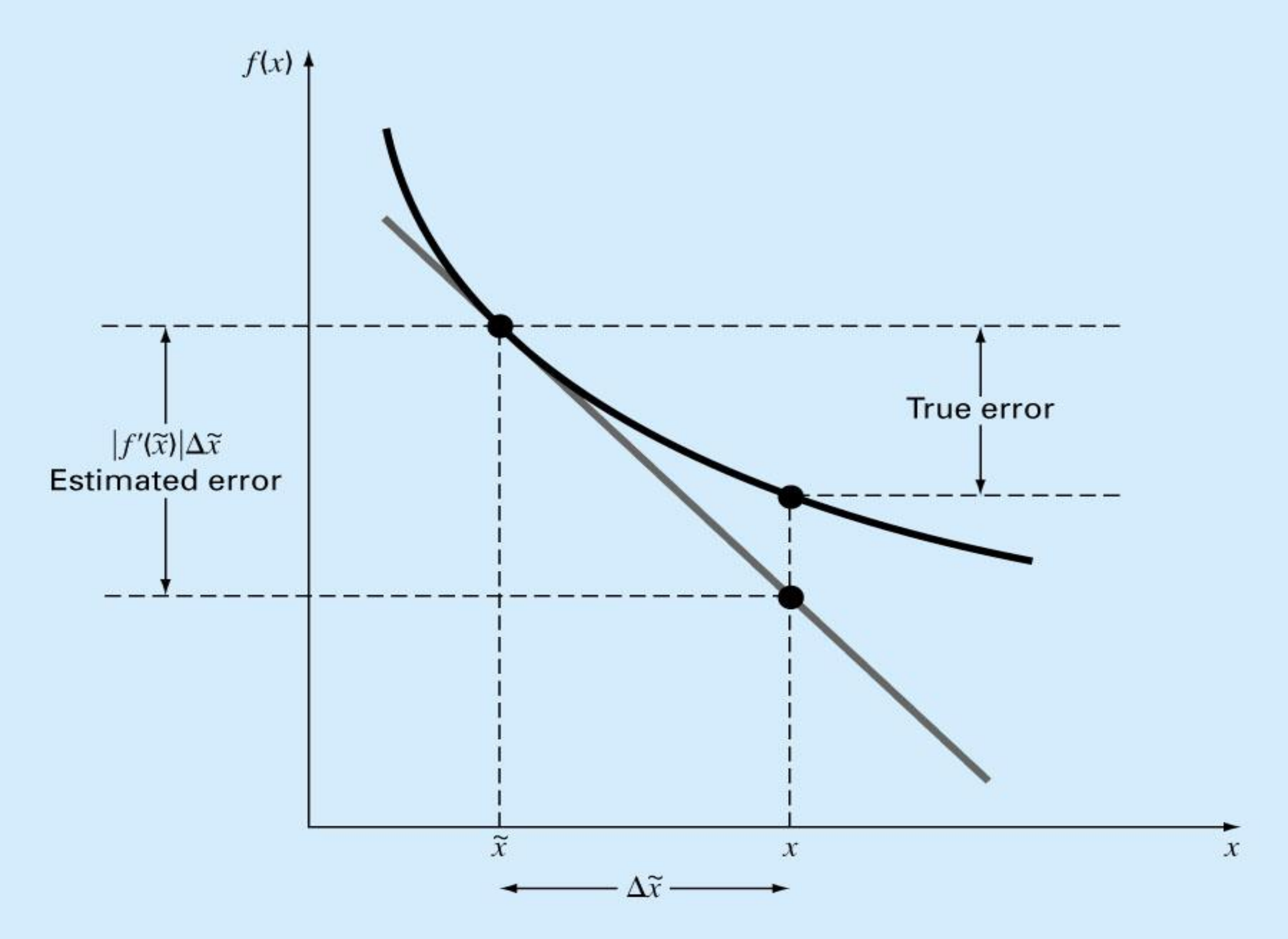
$$f(x_{i+1}, y_{i+1}) = f(x_i, y_i)$$

$$+\frac{\partial f}{\partial x}(x_{i+1} - x_i) + \frac{\partial f}{\partial y}(y_{i+1} - y_i)$$

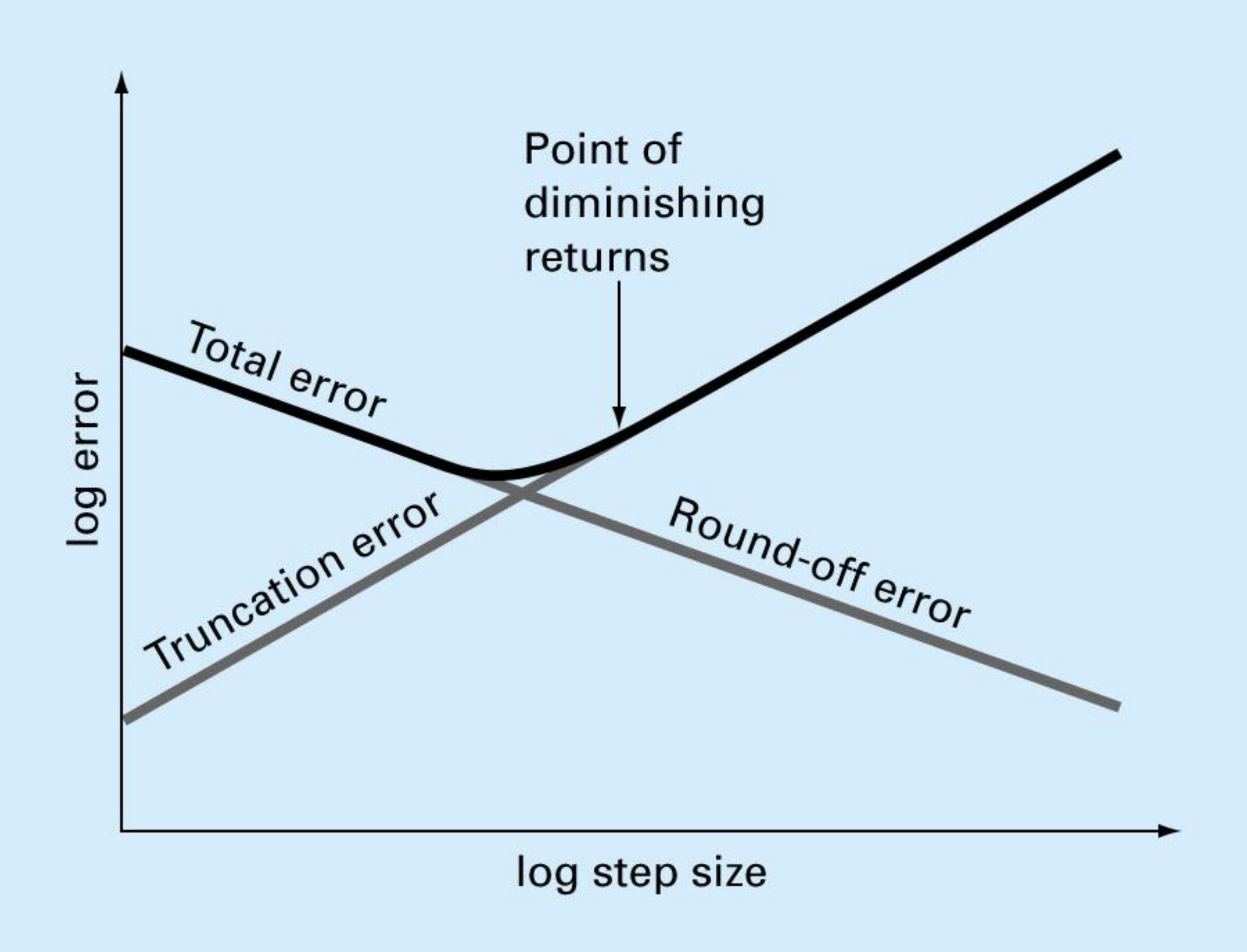
$$+\frac{1}{2!}\left[\frac{\partial^2 f}{\partial x^2}(x_{i+1} - x_i)^2 + 2\frac{\partial^2 f}{\partial x \partial y}(x_{i+1} - x_i)(y_{i+1} - y_i) + \frac{\partial^2 f}{\partial y^2}(y_{i+1} - y_i)^2\right]$$

$$+\cdots$$

ERROR PROPAGATION



TRADEOFF BETWEEN ROUND-OFF & TRUNCATION ERROR



HIGH ACCURACY DIFFERENTIATION FORMULAS

- High-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion.

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

$$f'(xi) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2}h + O(h^2)$$

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

$$f'(xi) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}h + O(h^2)$$

$$f'(xi) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$$

HIGH ACCURACY DIFFERENTIATION FORMULAS

- Inclusion of the 2nd derivative term has improved the accuracy to $O(h^2)$.
- Similar improved versions can be developed for the backward and centered formulas as well as for the approximations of the higher derivatives.

RICHARDSON EXTRAPOLATION

There are two ways to improve derivative estimates when employing finite divided differences:

Decrease the step size, or,

Use a higher-order formula that employs more points.

- A third approach, based on Richardson extrapolation, combines two derivative estimates to compute a third, more accurate approximation.

RICHARDSON EXTRAPOLATION

$$I \cong I(h_2) + \frac{1}{(h_1 / h_2)^2 - 1}[I(h_2) - I(h_1)]$$

$$h_2 = h_1 / 2$$

$$I \cong \frac{4}{3} I(h_2) - \frac{1}{3} I(h_1)]$$

$$\boxed{D \cong \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1)]}$$

- For centered difference approximations with $O(h^2)$.
- The application of this formula yield a new derivative estimate of $O(h^4)$.

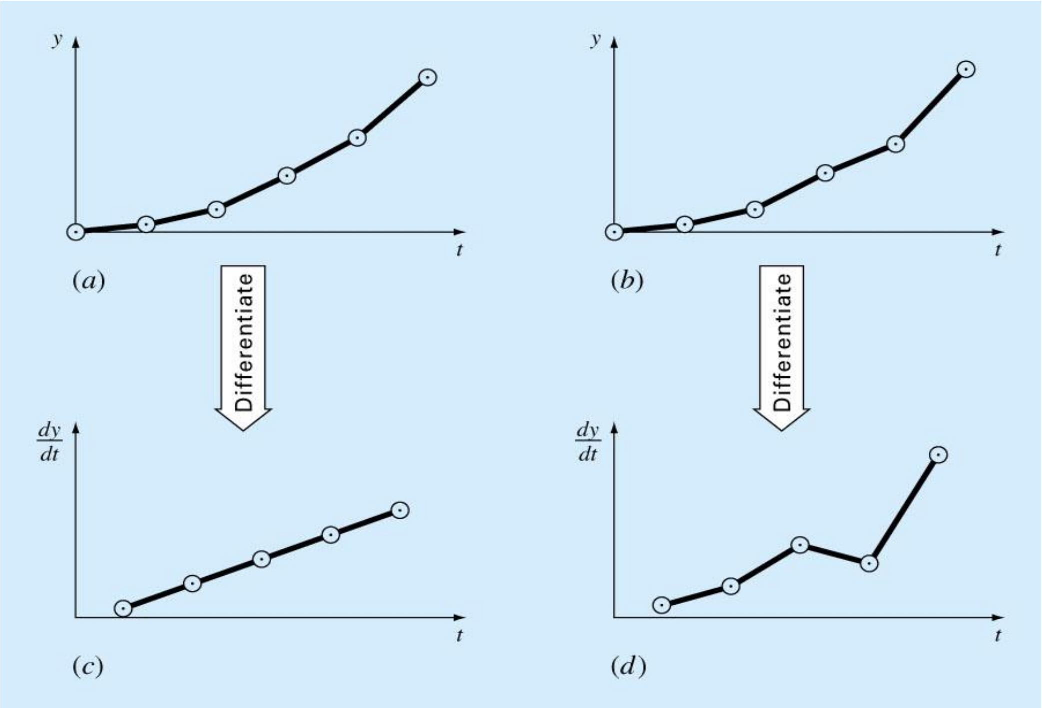
DERIVATIVES OF UNEQUALLY SPACED DATA

- Data from experiments or field studies are often collected at unequal intervals. One way to handle such data is to differentiate a 2nd-order Lagrange interpolating polynomial fit to three points:

$$f'(x) = f(x_{i-1})\frac{2x - x_i - x_{i+1}}{(x_{i-1} - x_i)\,(x_{i-1} - x_{i+1})} + f(x_i)\frac{2x - x_{i-1} - x_{i+1}}{(x_i - x_{i-1})\,(x_i - x_{i+1})} + f(x_{i+1})\frac{2x - x_{i-1} - x_i}{(x_{i+1} - x_{i-1})\,(x_{i+1} - x_i)}$$

where *x* is the value at which you want to estimate the derivative.

DERIVATIVES AND INTEGRALS FOR DATA WITH ERRORS



Because it is based on differences, differentiation tends to amplify data errors. Integration, which is based on summation, is very forgiving with regard to uncertain data because random positive and negative errors tend to cancel out.