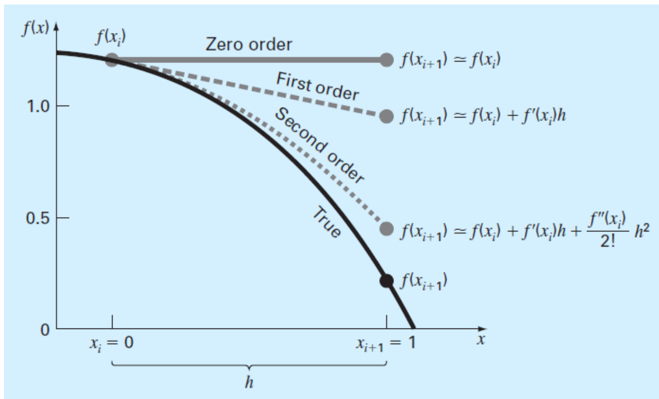
Lecture 04: Truncation Errors and Taylor Series



Truncation Errors

- Truncation errors are those that result from using an approximation in place of an exact mathematical procedure.

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

Taylor's Theorem

- Taylor's theorem and its associated formula, the Taylor series, is of great value in the study of numerical methods.
- In essence, the Taylor theorem states that any smooth function can be approximated as a polynomial.
- The *Taylor series* provides a means to predict a function value at one point in terms of the function value and its derivatives at another point.

Taylor's Theorem

- If the function *f* and its first *n*+1 derivatives are continuous on an interval containing *a* and *x*, then the value of the function at *x* is given by

$$
\begin{aligned}
f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 \\
+ \frac{f^{(3)}(a)}{3!}(x-a)^3 + \cdots \\
+ \frac{f^{(n)}(a)}{n!}(x-a)^n + R_n
\end{aligned}
$$

$$R_n = \int_a^x \frac{(x-t)^n}{n!} f^{(n+1)}(t)\,dt$$ where *t* = *a dummy variable.*

Integral form of remainder

Taylor's Theorem

- First Theorem of Mean for Integrals: If the function *g* is continuous and integrable on an interval containing *a* and *x*, then there exists a point *ξ* between *a* and *x* such that

$$\int_a^x g(t)\,dt = g(\xi)(x-a)$$

- Second Theorem of Mean for Integrals: If the functions *g* and *h* are continuous and integrable on an interval containing *a* and *x*, and *h* does not change sign in the interval, then there exists a point *ξ* between *a* and *x* such that

$$\int_a^x g(t)h(t)\,dt = g(\xi)\int_a^x h(t)\,dt$$

Taylor's Theorem

- Apply second theorem to R_n:

$$\int_a^x g(t)h(t)\,dt = g(\xi)\int_a^x h(t)\,dt$$

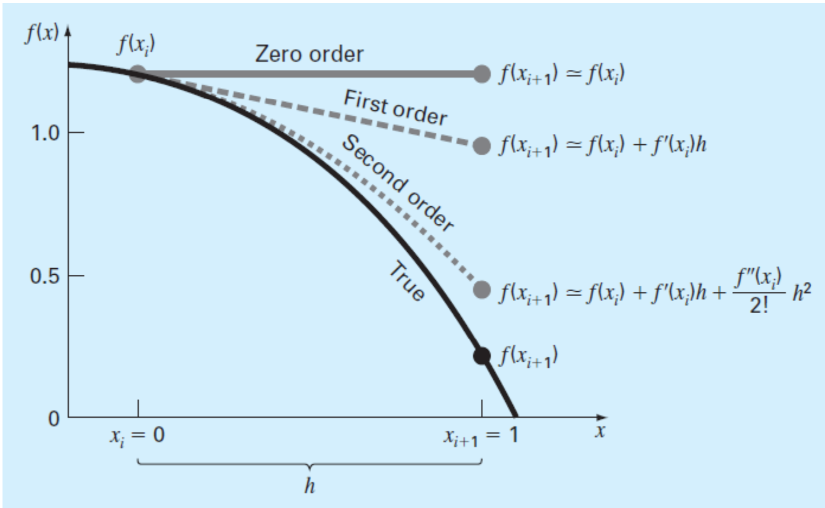
$$R_n = \int_a^x \frac{(x-t)^n}{n!} f^{(n+1)}(t)\,dt$$

$$g(t) = f^{(n+1)}(t) \qquad h(t) = \frac{(x-t)^n}{n!}$$

$$\boxed{R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-a)^{n+1}}$$

Derivative or Lagrange form of remainder

The Taylor Series



The Taylor Series

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

$$f''(x_{i+1}) \cong \frac{f'_f(x_i) - f'_b(x_i)}{\Delta x}$$

$$\boxed{f(h) \cong a_2h^2 + a_1h + a_0}$$

- Second-order Taylor series approximates the function with a second-order polynomial.

The Taylor Series

- Complete Taylor series expansion:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n$$

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

- ξ is a value of x that lies somewhere between x_i and x_{i+1}.
- There exists such a value that provides an exact determination of the error.

The Taylor Series

- In most cases, the inclusion of only a few terms will result in an approximation that is close enough to the true value for practical purposes.
- The assessment of how many terms are required to get "close enough" is based on the remainder term of the expansion.
- This relationship has two major drawbacks:
  - First, ξ is not known exactly but merely lies somewhere between x_i and x_{i+1}.
  - Second, to evaluate R_n, we need to determine the $(n + 1)$th derivative of $f(x)$. To do this, we need to know $f(x)$.

The Taylor Series

- Despite this dilemma, R_n is still useful for gaining insight into truncation errors.
- This is because we do have control over the term h in the equation.
- In other words, we can choose how far away from x we want to evaluate $f(x)$, and we can control the number of terms we include in the expansion.

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

- If the error is $O(h)$, halving the step size will halve the error.
- If the error is $O(h^2)$, halving the step size will quarter the error.

Example 1

Problem Statement. Use zero- through fourth-order Taylor series expansions to approximate the function

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

from $x_i = 0$ with $h = 1$. That is, predict the function's value at $x_{i+1} = 1$.

$$f(x_{i+1}) \simeq 1.2$$

$$E_t = 0.2 - 1.2 = -1.0$$

$$f'(0) = -0.4(0.0)^3 - 0.45(0.0)^2 - 1.0(0.0) - 0.25 = -0.25$$

$$f(x_{i+1}) \simeq 1.2 - 0.25h$$

Example 1

$$f(x_{i+1}) \simeq 1.2 - 0.25h$$

$$f(1) = 0.95.$$

$$E_t = 0.2 - 0.95 = -0.75$$

$$f''(0) = -1.2(0.0)^2 - 0.9(0.0) - 1.0 = -1.0$$

$$f(x_{i+1}) \simeq 1.2 - 0.25h - 0.5h^2$$

$$f(1) = 0.45$$

$$f(x) = 1.2 - 0.25h - 0.5h^2 - 0.15h^3 - 0.1h^4$$

$$R_4 = \frac{f^{(5)}(\xi)}{5!}h^5 = 0$$

Example 2

Problem Statement. Use Taylor series expansions with $n = 0$ to 6 to approximate $f(x) = \cos x$ at $x_{i+1} = \pi/3$ on the basis of the value of $f(x)$ and its derivatives at $x_i = \pi/4$. Note that this means that $h = \pi/3 - \pi/4 = \pi/12$.

$$f(\pi/3) = 0.5.$$

$$f\left(\frac{\pi}{3}\right) \cong \cos\left(\frac{\pi}{4}\right) = 0.707106781$$

$$\varepsilon_t = \left|\frac{0.5 - 0.707106781}{0.5}\right| 100\% = 41.4\%$$

Example 2

$$f\left(\frac{\pi}{3}\right) \cong \cos\left(\frac{\pi}{4}\right) - \sin\left(\frac{\pi}{4}\right)\left(\frac{\pi}{12}\right) = 0.521986659$$

$$|\varepsilon_t| = 4.40\%.$$

$$f\left(\frac{\pi}{3}\right) \cong \cos\left(\frac{\pi}{4}\right) - \sin\left(\frac{\pi}{4}\right)\left(\frac{\pi}{12}\right) - \frac{\cos(\pi/4)}{2}\left(\frac{\pi}{12}\right)^2 = 0.497754491$$

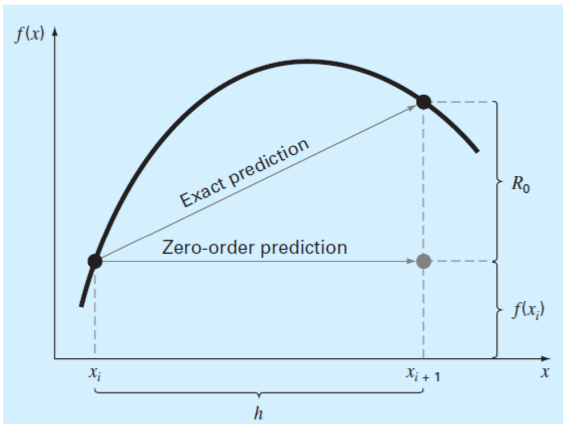
$$|\varepsilon_t| = 0.449\%.$$

Example 2

Order n	$f^{(n)}(x)$	$f(\pi/3)$	$\lvert\varepsilon_t\rvert$
0	$\cos x$	0.707106781	41.4
1	$-\sin x$	0.521986659	4.40
2	$-\cos x$	0.497754491	0.449
3	$\sin x$	0.499869147	2.62×10^{-2}
4	$\cos x$	0.500007551	1.51×10^{-3}
5	$-\sin x$	0.500000304	6.08×10^{-5}
6	$-\cos x$	0.499999988	2.44×10^{-6}

Remainder for Taylor Series Expansion

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



Remainder for Taylor Series Expansion

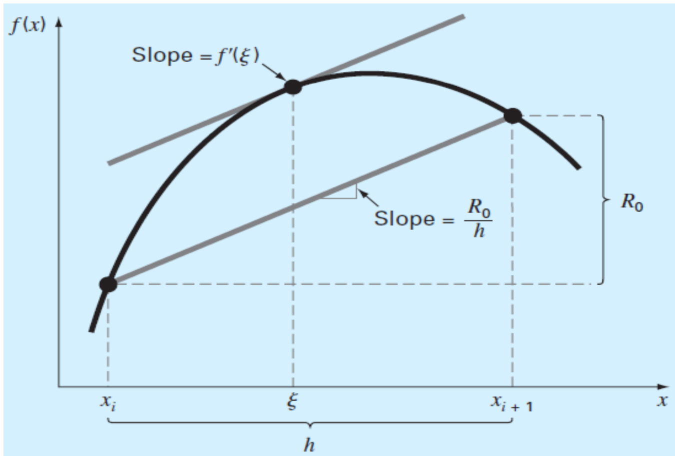
$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1}$$

$$R_0 = f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots$$

$$R_0 \cong f'(x_i)h$$

The derivative mean-value theorem states that if a function f(x) and its first derivative are continuous over an interval from x_i to x_{i+1}, then there exists at least one point on the function that has a slope, designated by $f'(\xi)$, that is parallel to the line joining $f(x_i)$ and $f(x_{i+1})$.

Remainder for Taylor Series Expansion



Remainder for Taylor Series Expansion

- A physical illustration of *derivative mean-value theorem* is that, if you travel between two points with an average velocity, there will be at least one moment during the course of the trip when you will be moving at that average velocity.

$$f'(\xi) = \frac{R_0}{h}$$

$$R_0 = f'(\xi)h$$

$$R_1 = \frac{f''(\xi)}{2!}h^2$$

Using Taylor Series to Estimate Truncation Errors

- Recall the bungee jumper problem: we were interested in determining *v*(*t*).

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

$$\Downarrow$$

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

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

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Using Taylor Series to Estimate Truncation Errors

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

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

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

The error of our derivative approximation should be proportional to the step size.

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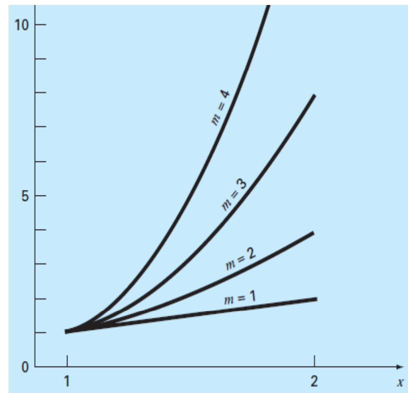
Example 3

- $f(x) = x^m$ for m = 1, 2, 3, and 4 over the range from x = 1 to 2. Notice that for $m = 1$ the function is linear, and as m increases, more curvature or nonlinearity is introduced into the function. Employ the first-order Taylor series to approximate this function for various values of the exponent m and the step size h.



Example 3

$$f(x_{i+1}) = f(x_i) + m x_i^{m-1} h$$

$$R_1 = \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \cdots$$

For $m = 1$, the actual value of the function at $x = 2$ is 2.

$$f(2) = 1 + 1(1) = 2 \qquad R_1 = 0$$

For $m = 2$, the actual value is $f(2) = 2^2 = 4$.

$$f(2) = 1 + 2(1) = 3$$

$$R_1 = \frac{2}{2}(1)^2 + 0 + 0 + \cdots = 1$$

Example 3

$$f(x_{i+1}) = f(x_i) + m x_i^{m-1} h$$

$$R_1 = \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \cdots$$

For $m = 3$, the actual value is $f(2) = 2^3 = 8$. The Taylor series approximation is

$$f(2) = 1 + 3(1)^2(1) = 4$$

and

$$R_1 = \tfrac{6}{2}(1)^2 + \tfrac{6}{6}(1)^3 + 0 + 0 + \cdots = 4$$

For $m = 4$, the actual value is $f(2) = 2^4 = 16$. The Taylor series approximation is

$$f(2) = 1 + 4(1)^3(1) = 5$$

and

$$R_1 = \tfrac{12}{2}(1)^2 + \tfrac{24}{6}(1)^3 + \tfrac{24}{24}(1)^4 + 0 + 0 + \cdots = 11$$

Example 3

$$f(x_{i+1}) = f(x_i) + m x_i^{m-1} h \qquad R_1 = \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \cdots$$

$$f(x + h) = f(x) + 4x_i^3 h$$

If $x = 1$, $f(1) = 1$ and this equation can be expressed as

$$f(1 + h) = 1 + 4h$$

with a remainder of

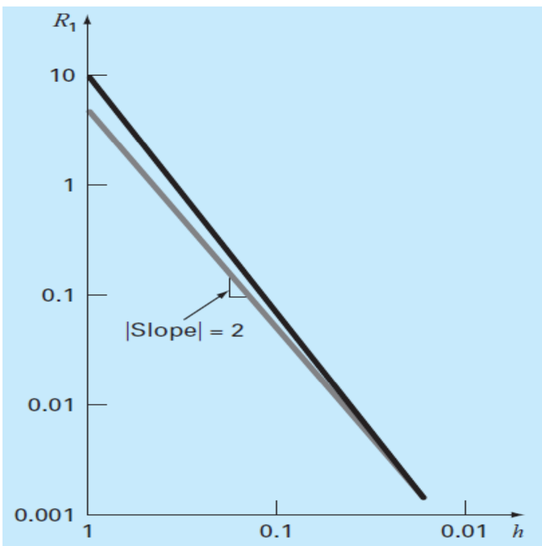
$$R_1 = 6h^2 + 4h^3 + h^4$$

- This leads to the conclusion that the discrepancy will decrease as *h is reduced.*
- *Also, at sufficiently* small values of *h, the error should become proportional to* h^2.

Example 3

h	True	First-Order Approximation	R_1
1	16	5	11
0.5	5.0625	3	2.0625
0.25	2.441406	2	0.441406
0.125	1.601807	1.5	0.101807
0.0625	1.274429	1.25	0.024429
0.03125	1.130982	1.125	0.005982
0.015625	1.063980	1.0625	0.001480

Example 3



Numerical Differentiation

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

- This equation has a label → *finite difference*.
- It can be represented generally as

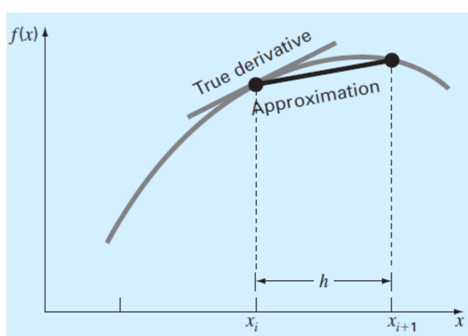
$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} + O(x_{i+1} - x_i)$$

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

Numerical Differentiation

$$\boxed{f'(x_i) = \frac{\Delta f_i}{h} + O(h)}$$

- Where f_i is referred to as the first forward difference.
- It is termed a "forward" difference because it utilizes data at *i* and *i*+1 to estimate the derivative .
- The entire term f/h is referred to as a **first finite divided difference**.



Backward Difference Approximation of First Derivative

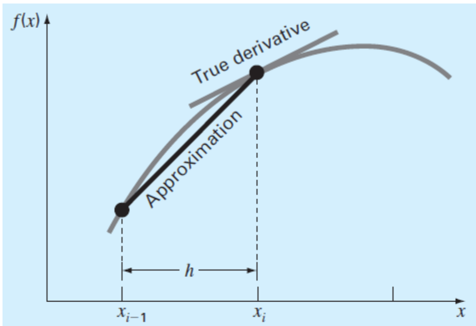
- The Taylor series can be expanded backward to calculate a previous value on the basis of a present value:

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

$$f'(x_i) \cong \frac{f(x_i) - f(x_{i-1})}{h} = \frac{\nabla f_1}{h}$$

- where the error is *O(h), and* ∇f_i is referred to as the *first backward difference*.

Backward Difference Approximation of First Derivative



Centered Difference Approximation of First Derivative

- A third way to approximate the first derivative is to subtract backward Taylor series expansion from the forward Taylor series expansion:

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

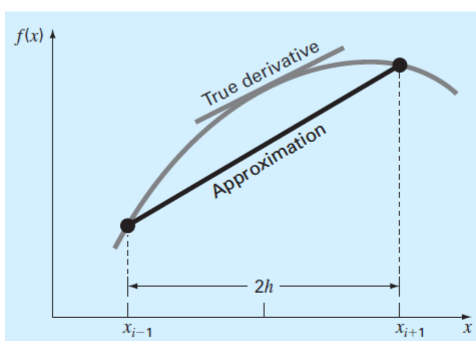
$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \cdots$$

$$\boxed{f(x_{i+1}) = f(x_{i-1}) + 2f'(x_i)h + 2\frac{f^{(3)}(x_i)}{3!}h^3 + \cdots}$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{f^{(3)}(x_i)}{6}h^2 + \cdots$$

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

Centered Difference Approximation of First Derivative



Example 4

Problem Statement. Use forward and backward difference approximations of $O(h)$ and a centered difference approximation of $O(h^2)$ to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ using a step size $h = 0.5$. Repeat the computation using $h = 0.25$. Note that the derivative can be calculated directly as

$$f'(x) = -0.4x^3 - 0.45x^2 - 1.0x - 0.25$$

and can be used to compute the true value as $f'(0.5) = -0.9125$.

Example 4

Solution. For $h = 0.5$, the function can be employed to determine

$$\begin{aligned} x_{i-1} &= 0 & f(x_{i-1}) &= 1.2 \\ x_i &= 0.5 & f(x_i) &= 0.925 \\ x_{i+1} &= 1.0 & f(x_{i+1}) &= 0.2 \end{aligned}$$

These values can be used to compute the forward divided difference [Eq. (4.17)],

$$f'(0.5) \cong \frac{0.2 - 0.925}{0.5} = -1.45 \qquad |\varepsilon_t| = 58.9\%$$

the backward divided difference [Eq. (4.20)],

$$f'(0.5) \cong \frac{0.925 - 1.2}{0.5} = -0.55 \qquad |\varepsilon_t| = 39.7\%$$

and the centered divided difference [Eq. (4.22)],

$$f'(0.5) \cong \frac{0.2 - 1.2}{1.0} = -1.0 \qquad |\varepsilon_t| = 9.6\%$$

Example 4

For $h = 0.25$,

$$\begin{aligned} x_{i-1} &= 0.25 & f(x_{i-1}) &= 1.10351563 \\ x_i &= 0.5 & f(x_i) &= 0.925 \\ x_{i+1} &= 0.75 & f(x_{i+1}) &= 0.63632813 \end{aligned}$$

which can be used to compute the forward divided difference,

$$f'(0.5) \cong \frac{0.63632813 - 0.925}{0.25} = -1.155 \qquad |\varepsilon_t| = 26.5\%$$

the backward divided difference,

$$f'(0.5) \cong \frac{0.925 - 1.10351563}{0.25} = -0.714 \qquad |\varepsilon_t| = 21.7\%$$

and the centered divided difference,

$$f'(0.5) \cong \frac{0.63632813 - 1.10351563}{0.5} = -0.934 \qquad |\varepsilon_t| = 2.4\%$$

Finite Difference Approximations of Higher Derivatives

- Besides first derivatives, the Taylor series expansion can be used to derive numerical estimates of higher derivatives.
- We write a forward Taylor series expansion for $f(x_{i+2})$ in terms of $f(x_i)$:

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

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

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

Finite Difference Approximations of Higher Derivatives

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

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

- This relationship is called the *second forward finite divided difference.*
- *Similar manipulations* can be employed to derive a backward version and a centered version.

Finite Difference Approximations of Higher Derivatives

- Backward version

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

- Centered version

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

- The centered version can be alternatively expressed as

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

Error Propagation

- **Functions of a Single Variable**

$$\boxed{\Delta f(\tilde{x}) = |f(x) - f(\tilde{x})|}$$

$$f(x) = f(\tilde{x}) + f'(\tilde{x})(x - \tilde{x}) + \frac{f''(\tilde{x})}{2}(x - \tilde{x})^2 + \cdots$$

$$\boxed{f(x) - f(\tilde{x}) \cong f'(\tilde{x})(x - \tilde{x})}$$

$$\boxed{\Delta f(\tilde{x}) = |f'(\tilde{x})|\Delta \tilde{x}}$$

Example 5

Problem Statement. Given a value of $\tilde{x} = 2.5$ with an error of $\Delta\tilde{x} = 0.01$, estimate the resulting error in the function, $f(x) = x^3$.

Solution. Using Eq. (4.25),

$$\Delta f(\tilde{x}) \cong 3(2.5)^2(0.01) = 0.1875$$

Because $f(2.5) = 15.625$, we predict that

$$f(2.5) = 15.625 \pm 0.1875$$

Error Propagation

- **Functions of More than One Variable**
  - Multivariable version of the Taylor series

$$f(u_{i+1}, v_{i+1}) = f(u_i, v_i) + \frac{\partial f}{\partial u}(u_{i+1} - u_i) + \frac{\partial f}{\partial v}(v_{i+1} - v_i)$$
$$+ \frac{1}{2!}\left[\frac{\partial^2 f}{\partial u^2}(u_{i+1} - u_i)^2 + 2\frac{\partial^2 f}{\partial u \partial v}(u_{i+1} - u_i)(v_{i+1} - v_i)\right.$$
$$\left.+ \frac{\partial^2 f}{\partial v^2}(v_{i+1} - v_i)^2\right] + \cdots$$

Error Propagation

- **Functions of More than One Variable**

$$\boxed{\Delta f(\tilde{u}, \tilde{v}) = \left|\frac{\partial f}{\partial u}\right| \Delta\tilde{u} + \left|\frac{\partial f}{\partial v}\right| \Delta\tilde{v}}$$

$$\boxed{\Delta f(\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_n) \cong \left|\frac{\partial f}{\partial x_1}\right| \Delta\tilde{x}_1 + \left|\frac{\partial f}{\partial x_2}\right| \Delta\tilde{x}_2 + \cdots + \left|\frac{\partial f}{\partial x_n}\right| \Delta\tilde{x}_n}$$

Error Propagation

- **Functions of More than One Variable**

$$\Delta f(\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_n) \cong \left|\frac{\partial f}{\partial x_1}\right| \Delta \tilde{x}_1 + \left|\frac{\partial f}{\partial x_2}\right| \Delta \tilde{x}_2 + \cdots + \left|\frac{\partial f}{\partial x_n}\right| \Delta \tilde{x}_n$$

- Estimated error bounds associated with common mathematical operations using inexact numbers

Operation		Estimated Error
Addition	$\Delta(\tilde{u} + \tilde{v})$	$\Delta\tilde{u} + \Delta\tilde{v}$
Subtraction	$\Delta(\tilde{u} - \tilde{v})$	$\Delta\tilde{u} + \Delta\tilde{v}$
Multiplication	$\Delta(\tilde{u} \times \tilde{v})$	$\lvert\tilde{u}\rvert\Delta\tilde{v} + \lvert\tilde{v}\rvert\Delta\tilde{u}$
Division	$\Delta\left(\frac{\tilde{u}}{\tilde{v}}\right)$	$\frac{\lvert\tilde{u}\rvert\Delta\tilde{v} + \lvert\tilde{v}\rvert\Delta\tilde{u}}{\lvert\tilde{v}\rvert^2}$

Example 6

Problem Statement. The deflection y of the top of a sailboat mast is

$$y = \frac{FL^4}{8EI}$$

where F = a uniform side loading (N/m), L = height (m), E = the modulus of elasticity (N/m^2), and I = the moment of inertia (m^4). Estimate the error in y given the following data:

$\tilde{F} = 750$ N/m $\quad\quad \Delta\tilde{F} = 30$ N/m

$\tilde{L} = 9$ m $\quad\quad \Delta\tilde{L} = 0.03$ m

$\tilde{E} = 7.5 \times 10^9$ N/m^2 $\quad\quad \Delta\tilde{E} = 5 \times 10^7$ N/m^2

$\tilde{I} = 0.0005$ m^4 $\quad\quad \Delta\tilde{I} = 0.000005$ m^4

Example 6

Solution. Employing Eq. (4.27) gives

$$\Delta y(\tilde{F}, \tilde{L}, \tilde{E}, \tilde{I}) = \left|\frac{\partial y}{\partial F}\right| \Delta \tilde{F} + \left|\frac{\partial y}{\partial L}\right| \Delta \tilde{L} + \left|\frac{\partial y}{\partial E}\right| \Delta \tilde{E} + \left|\frac{\partial y}{\partial I}\right| \Delta \tilde{I}$$

or

$$\Delta y(\tilde{F}, \tilde{L}, \tilde{E}, \tilde{I}) \cong \frac{\tilde{L}^4}{8\tilde{E}\tilde{I}} \Delta \tilde{F} + \frac{\tilde{F}\tilde{L}^3}{2\tilde{E}\tilde{I}} \Delta \tilde{L} + \frac{\tilde{F}\tilde{L}^4}{8\tilde{E}^2\tilde{I}} \Delta \tilde{E} + \frac{\tilde{F}\tilde{L}^4}{8\tilde{E}\tilde{I}^2} \Delta \tilde{I}$$

$$\Delta y = 0.006561 + 0.002187 + 0.001094 + 0.00164 = 0.011482$$

$$\boxed{y = 0.164025 \pm 0.011482.}$$

$$y_{min} = \frac{720(8.97)^4}{8(7.55 \times 10^9)0.000505} = 0.152818 \qquad y_{max} = \frac{780(9.03)^4}{8(7.45 \times 10^9)0.000495} = 0.175790$$

Stability and Condition

- The condition of a mathematical problem relates to its sensitivity to changes in its input values.
- A computation is numerically unstable if the uncertainty of the input values is grossly magnified by the numerical method.

$$f(x) = f(\tilde{x}) + f'(\tilde{x})(x - \tilde{x})$$

$$\boxed{\frac{f(x) - f(\tilde{x})}{f(x)} \cong \frac{f'(\tilde{x})(x - \tilde{x})}{f(\tilde{x})}}$$ Relative error of $f(x)$

$$\boxed{\frac{x - \tilde{x}}{\tilde{x}}}$$ Relative error of x

Stability and Condition

- A condition number can be defined as the ratio of these relative errors

$$\text{Condition number} = \frac{\tilde{x} f'(\tilde{x})}{f(\tilde{x})}$$

- A value of 1 tells us that the function's relative error is identical to the relative error in *x*.
- A value greater than 1 tells us that the relative error is amplified, whereas a value less than 1 tells us that it is attenuated.
- Functions with very large values are said to be ill-conditioned

Example 7

Problem Statement. Compute and interpret the condition number for

$$f(x) = \tan x \qquad \text{for } \tilde{x} = \frac{\pi}{2} + 0.1\left(\frac{\pi}{2}\right)$$

$$f(x) = \tan x \qquad \text{for } \tilde{x} = \frac{\pi}{2} + 0.01\left(\frac{\pi}{2}\right)$$

Solution. The condition number is computed as

$$\text{Condition number} = \frac{\tilde{x}(1/\cos^2 x)}{\tan \tilde{x}}$$

Example 7

For $\tilde{x} = \pi/2 + 0.1(\pi/2)$,

$$\text{Condition number} = \frac{1.7279(40.86)}{-6.314} = -11.2$$

Thus, the function is ill-conditioned. For $\tilde{x} = \pi/2 + 0.01(\pi/2)$, the situation is even worse:

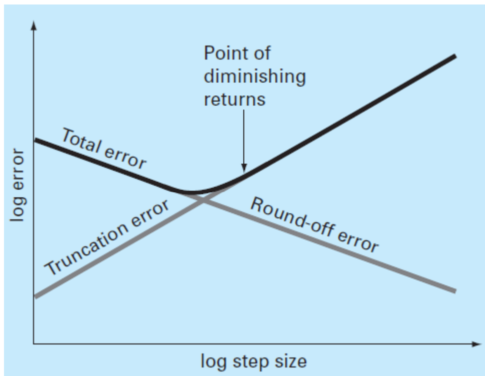
$$\text{Condition number} = \frac{1.5865(4053)}{-63.66} = -101$$

Total Numerical Error

- The total numerical error is the summation of the truncation and round-off errors.
- In general, the only way to minimize round-off errors is to increase the number of significant figures of the computer.
- Further, we have noted that round-off error may increase due to subtractive cancellation or due to an increase in the number of computations in an analysis.
- In contrast, truncation error can be reduced by decreasing the step size.
- Because a decrease in step size can lead to subtractive cancellation or to an increase in computations, the truncation errors are decreased as the round-off errors are increased.

Total Numerical Error

- Therefore, we are faced by a dilemma.
- In a computation, we could conceivably decrease the step size to minimize truncation errors only to discover that in doing so, the round-off error begins to dominate the solution and the total error grows!



Total Numerical Error

- Therefore, the challenge is to determine an appropriate step size for a particular computation.
- We would like to choose a large step size in order to decrease the amount of calculations and round-off errors without incurring the penalty of a large truncation error.
- The challenge is to identify the point of diminishing returns where round-off error begins to negate the benefits of step-size reduction.
- When using MATLAB, such situations are relatively uncommon because of its 15- to 16-digit precision.

Total Numerical Error

- However, they sometimes do occur and suggest a sort of "numerical uncertainty principle".
- It places an absolute limit on the accuracy that may be obtained using certain computerized numerical methods.

Error Analysis of Numerical Differentiation

$$f'(x_i) = \underbrace{\frac{f(x_{i+1}) - f(x_{i-1})}{2h}}_{\text{Finite-difference approximation}} - \underbrace{\frac{f^{(3)}(\xi)}{6}h^2}_{\text{Truncation error}}$$

True value

- If the two function values in the numerator of the finite-difference approximation have no round-off error, the only error is due to truncation.
- However, because we are using digital computers, the function values do include round-off error as in

$$f(x_{i-1}) = \tilde{f}(x_{i-1}) + e_{i-1}$$
$$f(x_{i+1}) = \tilde{f}(x_{i+1}) + e_{i+1}$$

Error Analysis of Numerical Differentiation

$$f'(x_i) = \frac{\tilde{f}(x_{i+1}) - \tilde{f}(x_{i-1})}{2h} + \frac{e_{i+1} - e_{i-1}}{2h} - \frac{f^{(3)}(\xi)}{6}h^2$$

True value | Finite-difference approximation | Round-off error | Truncation error

- Assuming that the absolute value of each component of the round-off error has an upper bound of ε, the maximum possible value of the difference $e_{i+1} - e_{i-1}$ will be 2ε.
- Further, assume that the third derivative has a maximum absolute value of *M.*

Error Analysis of Numerical Differentiation

- An upper bound on the absolute value of the total error can therefore be represented as

$$\text{Total error} = \left| f'(x_i) - \frac{\tilde{f}(x_{i+1}) - \tilde{f}(x_{i-1})}{2h} \right| \le \frac{\varepsilon}{h} + \frac{h^2 M}{6}$$

$$\boxed{h_{\text{opt}} = \sqrt[3]{\frac{3\varepsilon}{M}}}$$

Example 8

Problem Statement. In Example 4.4, we used a centered difference approximation of $O(h^2)$ to estimate the first derivative of the following function at $x = 0.5$,

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

Perform the same computation starting with $h = 1$. Then progressively divide the step size by a factor of 10 to demonstrate how round-off becomes dominant as the step size is reduced. Relate your results to Eq. (4.31). Recall that the true value of the derivative is -0.9125.

$$\boxed{h_{\text{opt}} = \sqrt[3]{\frac{3\varepsilon}{M}}}$$

$$M = |f^3(0.5)| = |-2.4(0.5) - 0.9| = 2.1$$

$$\varepsilon = 0.5 \times 10^{-16}$$

$$h_{\text{opt}} = \sqrt[3]{\frac{3(0.5 \times 10^{-16})}{2.1}} = 4.3 \times 10^{-6}$$

Control of Numerical Errors

- First and foremost, avoid subtracting two nearly equal numbers.
- Sometimes you can rearrange or reformulate the problem to avoid subtractive cancellation.
- If this is not possible, you may want to use extended-precision arithmetic.
- Furthermore, when adding and subtracting numbers, it is best to sort the numbers and work with the smallest numbers first. This avoids loss of significance.

Control of Numerical Errors

- The Taylor series is our primary tool for analysis of both truncation and round-off errors.
- The tendency is to push forward with the numerical computations and try to estimate the accuracy of your results.
- This can sometimes be done by seeing if the results satisfy some condition or equation as a check.
- Or it may be possible to substitute the results back into the original equation to check that it is actually satisfied.
- Finally you should be prepared to perform numerical experiments to increase your awareness of computational errors and possible ill-conditioned problems.

Blunders, Formulation Errors, and Data Uncertainty

- Blunders → gross errors.
- Most blunders must be attributed to human imperfection.
- Formulation, or model, errors relate to bias that can be ascribed to incomplete mathematical models.
- Data Uncertainty → Errors sometimes enter into an analysis because of uncertainty in the physical data upon which a model is based.

Assignment-04

- Problems 4.1, 4.4, 4.7, 4.8, 4.9, 4.17, 4.20