Theoritical Models for Computing: Errors & Taylor Series

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Part A

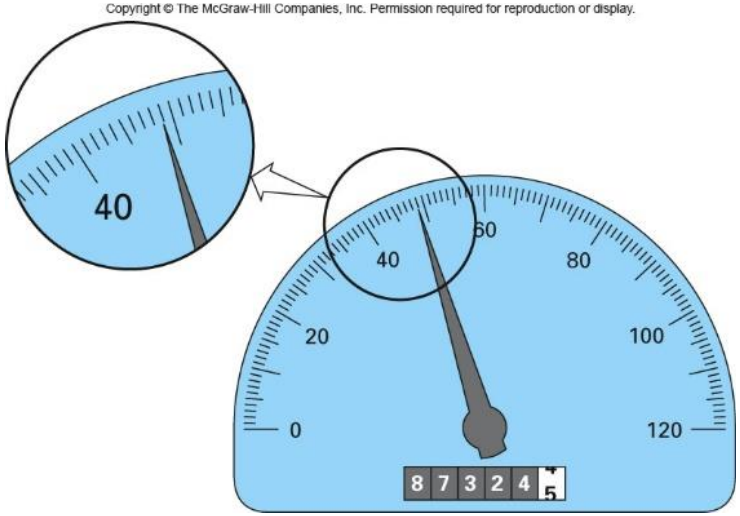
ACCURACY, ERROR & APPROXIMATE ERROR

Motivations

We ask for numerical methods since we cannot get exact solution !!

Numerical methods only provide approximate results, not exact ones.

So how we confident our results obtained from numerical methods ????



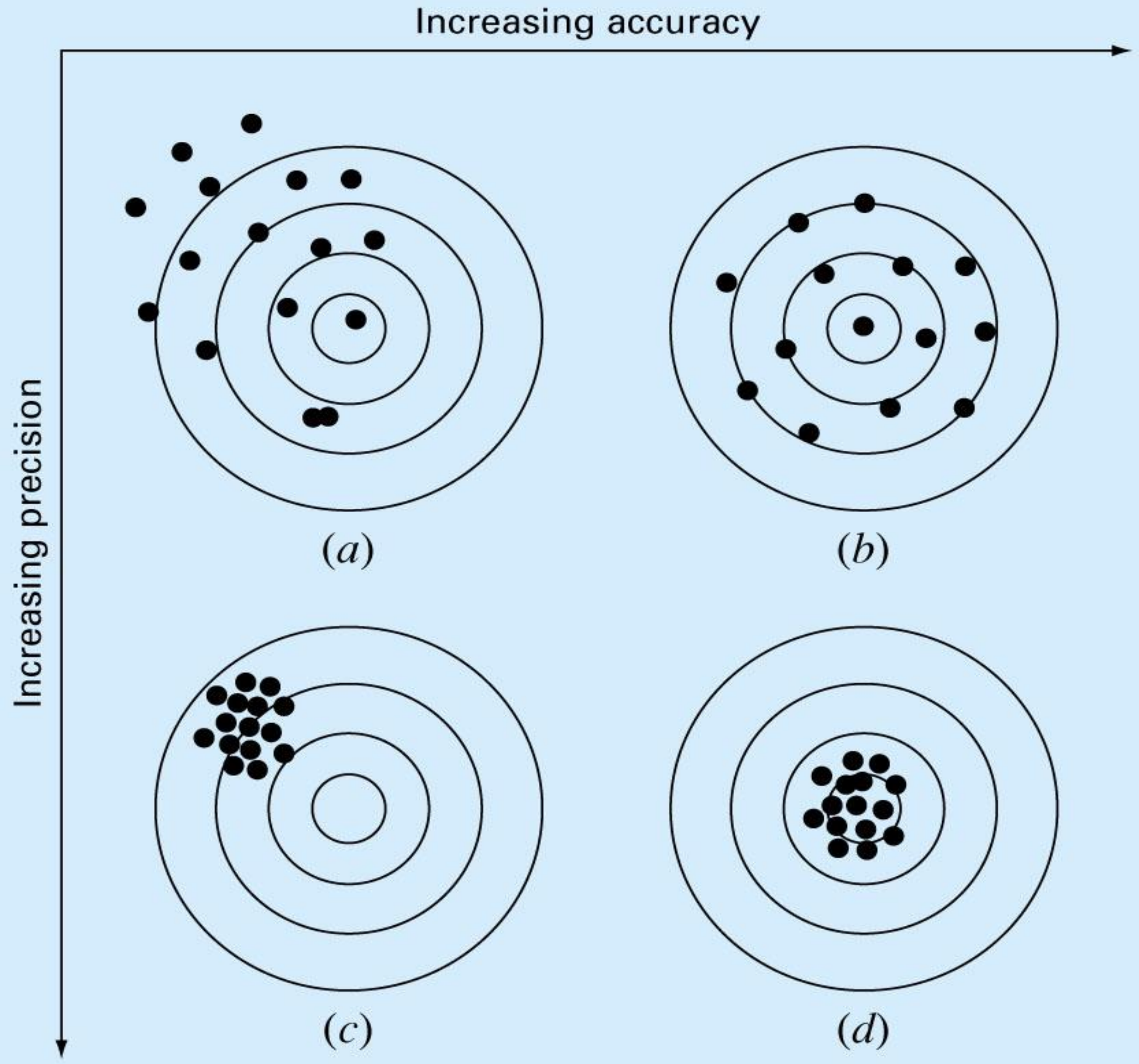
$\boldsymbol{x} = \sqrt{\mathbf{2}} = 1.41421356237\ldots$

Accuracy and Precision

- Errors associated with both **calculations** and **measurements** can be characterized with regard to their accuracy and precision

- **Accuracy** refers to how closely a **computed or measured value** agrees with the **true value**

- **Precision** refers to how closely **individual computed or measured values** agree with **each other**


Increasing accuracy
Increasing precision
(a)
(b)
(c)
(d)

Objectives

Errors

Round-off errors

Approximate errors

1. Error Definitions

Error, or true error E_t, is defined as the difference between the true value in a calculation and the approximate value found using a numerical method etc.

True Error E_t = True Value – Approximate Value

Example

The derivative, $f'(x)$ of a function $f(x)$ can be approximated by the equation,

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

If $f(x) = 7e^{0.5x}$ and $h = 0.3$

a) Find the approximate value of $f'(2)$

b) True value of $f'(2)$

c) Error for part (a)

Example (cont.)

Solution:

a) For $x = 2$ and $h = 0.3$

$$f'(2) \approx \frac{f(2+0.3) - f(2)}{0.3}$$

$$= \frac{f(2.3) - f(2)}{0.3}$$

$$= \frac{7e^{0.5(2.3)} - 7e^{0.5(2)}}{0.3}$$

$$= \frac{22.107 - 19.028}{0.3} = 10.263$$

Example (cont.)

Solution:

b) The exact value of $f'(2)$ can be found by using our knowledge of differential calculus.

$$f(x) = 7e^{0.5x}$$

$$f'(x) = 7 \times 0.5 \times e^{0.5x}$$

$$= 3.5e^{0.5x}$$

So the true value of $f'(2)$ is

$$f'(2) = 3.5e^{0.5(2)}$$

$$= 9.5140$$

Error is calculated as

$$E_t = \text{ True Value – Approximate Value}$$

$$= 9.5140 - 10.263 = -0.722$$

2. Relative Error

Defined as the ratio between the true error, and the true value.

$$\text{Relative True Error } (\varepsilon_t) = \frac{\text{True Error}}{\text{True Value}}$$

Example - Relative True Error

Following from the previous example for true error, find the relative true error for $f(x) = 7e^{0.5x}$ at $f'(2)$ with $h = 0.3$

From the previous example,

$$E_t = -0.722$$

Relative True Error is defined as

$$\varepsilon_t = \frac{\text{True Error}}{\text{True Value}}$$

$$= \frac{-0.722}{9.5140} = -0.075888$$

as a percentage,

$$\varepsilon_t = -0.075888 \times 100\% = -7.5888\%$$

3. Approximate Error

What can be done if true values are not known or are very difficult to obtain?

Approximate error is defined as the difference between the present approximation and the previous approximation.

Approximate Error (E_a) = Present Approximation

– Previous Approximation

Example - Approximate Error

For $f(x) = 7e^{0.5x}$ at $x = 2$ find the following,

a) $f'(2)$ using $h = 0.3$

b) $f'(2)$ using $h = 0.15$

c) approximate error for the value of $f'(2)$ for part b)

Solution:

a) For $x = 2$ and $h = 0.3$

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

$$f'(2) \approx \frac{f(2+0.3) - f(2)}{0.3}$$

Example (cont.)

Solution: (cont.)

$$= \frac{f(2.3) - f(2)}{0.3}$$

$$= \frac{7e^{0.5(2.3)} - 7e^{0.5(2)}}{0.3}$$

$$= \frac{22.107 - 19.028}{0.3} = 10.263$$

b) For $x = 2$ and $h = 0.15$

$$f^{'}(2) \approx \frac{f(2+0.15) - f(2)}{0.15}$$

$$= \frac{f(2.15) - f(2)}{0.15}$$

Example (cont.)

Solution: (cont.)

$$= \frac{7e^{0.5(2.15)} - 7e^{0.5(2)}}{0.15}$$

$$= \frac{20.50 - 19.028}{0.15} = 9.8800$$

c) So the approximate error, E_a is

$$E_a = \text{Present Approximation} - \text{Previous Approximation}$$

$$= 9.8800 - 10.263$$

$$= -0.38300$$

4. Relative Approximate Error

Defined as the ratio between the approximate error and the present approximation.

$$\text{Relative Approximate Error } (\varepsilon_a) = \frac{\text{Approximate Error}}{\text{Present Approximation}}$$

Example - Relative Approximate Error

For $f(x) = 7e^{0.5x}$ at $x = 2$, find the relative approximate error using values from $h = 0.3$ and $h = 0.15$

Solution:

From Example 3, the approximate value of $f'(2) = 10.263$ using $h = 0.3$ and $f'(2) = 9.8800$ using $h = 0.15$

$$E_a = \text{Present Approximation} - \text{Previous Approximation}$$

$$= 9.8800 - 10.263$$

$$= -0.38300$$

Example (cont.)

Solution: (cont.)

$$\varepsilon_a = \frac{\text{Approximate Error}}{\text{Present Approximation}}$$

$$= \frac{-0.38300}{9.8800} = -0.038765$$

as a percentage,

$$\varepsilon_a = -0.038765 \times 100\% = -3.8765\%$$

Absolute relative approximate errors may also need to be calculated,

$$|\varepsilon_a| = |-0.038765| = 0.038765 \text{ or } 3.8765\%$$

How is Absolute Relative Error used as a stopping criterion?

If $|\varepsilon_a| < \varepsilon_s$ where ε_s is a pre-specified tolerance, then no further iterations are necessary and the process is stopped.

If *at least n significant digits/figures* are required to be correct in the result, then

$$\varepsilon_s = (0.5 \times 10^{(2-n)})\%$$

Table of Values

For $f(x) = 7e^{0.5x}$ at $x = 2$ with varying step size, h

h	$f'(2)$	$\lvert\varepsilon_a\rvert$	n
0.3	10.263	N/A	0
0.15	9.8800	0.038765%	3
0.10	9.7558	0.012731%	3
0.01	9.5378	0.024953%	3
0.001	9.5164	0.002248%	4

5. Round-off Errors

Numbers such as Pi, e, or $\sqrt{7}$ cannot be expressed by a fixed number of significant figures.

Computers use a base-2 representation, they cannot precisely represent certain exact base-10 numbers.

Fractional quantities are typically represented in computer using **“floating point” form**, e.g.,

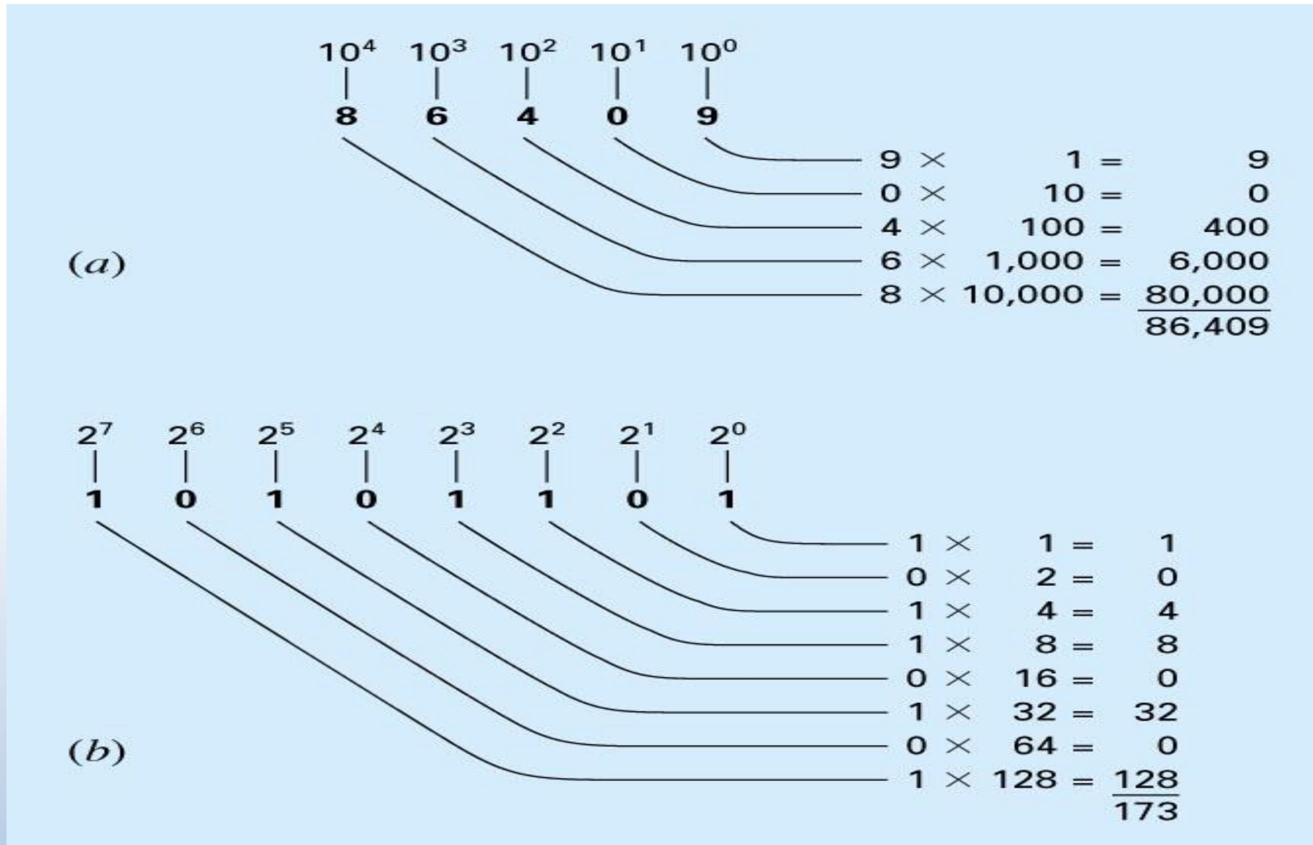
Integer part

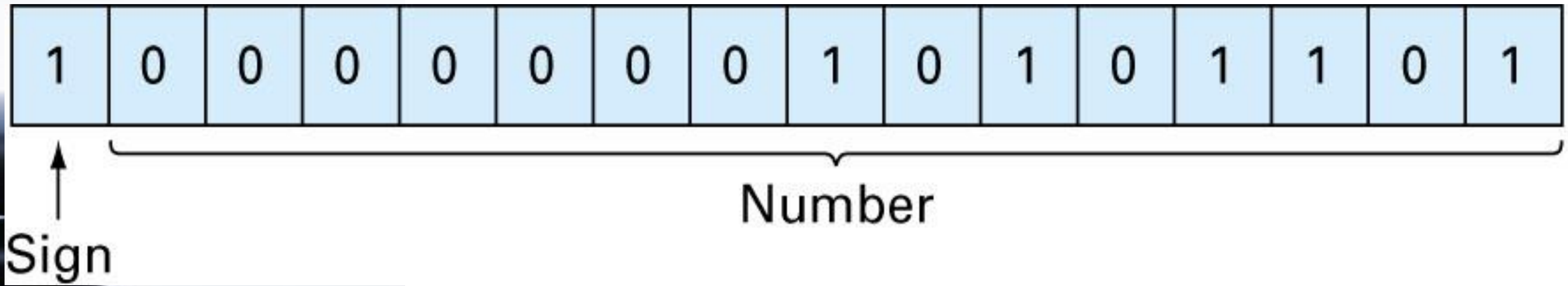
exponent

$$m.\boxed{b^e}$$

mantissa

Base of the number system used


(a)
10^4 10^3 10^2 10^1 10^0
8 6 4 0 9
9 × 1 = 9
0 × 10 = 0
4 × 100 = 400
6 × 1,000 = 6,000
8 × 10,000 = 80,000
86,409
(b)
2^7 2^6 2^5 2^4 2^3 2^2 2^1 2^0
1 0 1 0 1 1 0 1
1 × 1 = 1
0 × 2 = 0
1 × 4 = 4
1 × 8 = 8
0 × 16 = 0
1 × 32 = 32
0 × 64 = 0
1 × 128 = 128
173


1
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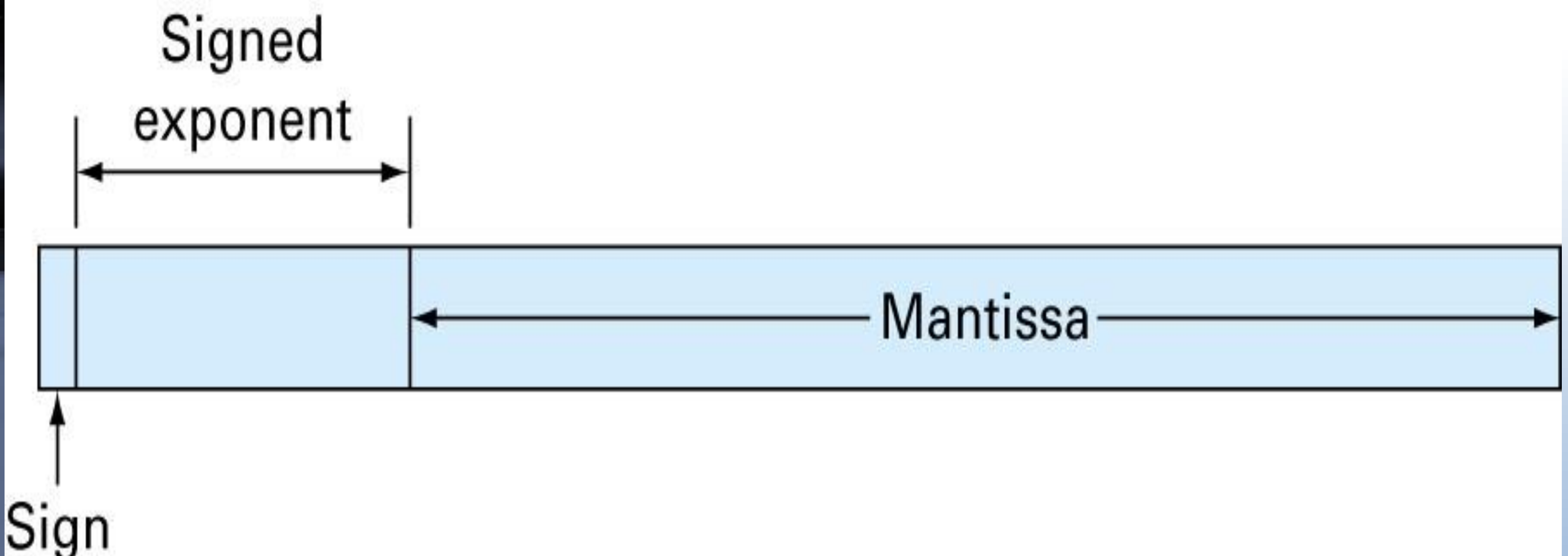
Number
Sign


Signed
exponent
Mantissa
Sign

156.78 ▶▶ 0.15678×10^3 in a floating point base-10 system

$$\frac{1}{34} = 0.029411765$$

Suppose only 4 decimal places to be stored

$$0.0294 \times 10^0 \qquad \frac{1}{2} \le |m| < 1$$

Normalized to remove the leading zeroes. Multiply the mantissa by 10 and lower the exponent by 1

$0.294\underline{1} \times 10^{-1}$

Additional significant figure is retained

$$\frac{1}{b} \leq |m| < 1$$

Therefore

for a base-10 system $0.1 \leq m < 1$

for a base-2 system $0.5 \leq m < 1$

Floating point representation allows both fractions and very large numbers to be expressed on the computer. However,

- Floating point numbers take up more room.
- Take longer to process than integer numbers.
- Round-off errors are introduced because mantissa holds only a finite number of significant figures.

Chopping

Example:

π=3.14159265358

to be stored on a base-10 system carrying 7 significant digits π=3.141592 => chopping error

ε_t=0.00000065

If rounded π=3.141593 => round-off error

ε_t=0.00000035

Some machines use chopping, because rounding adds to the computational overhead. Since number of significant figures is large enough, resulting chopping error is negligible.

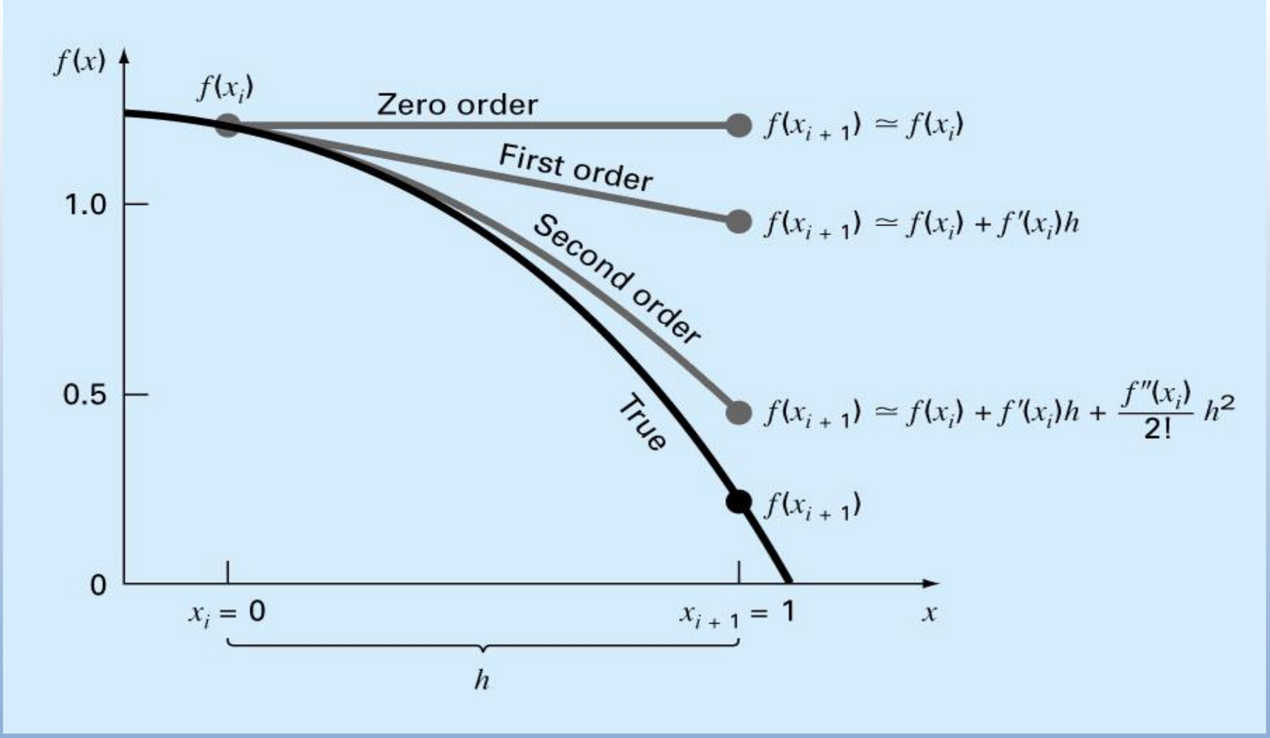
PART B

TAYLOR SERIES

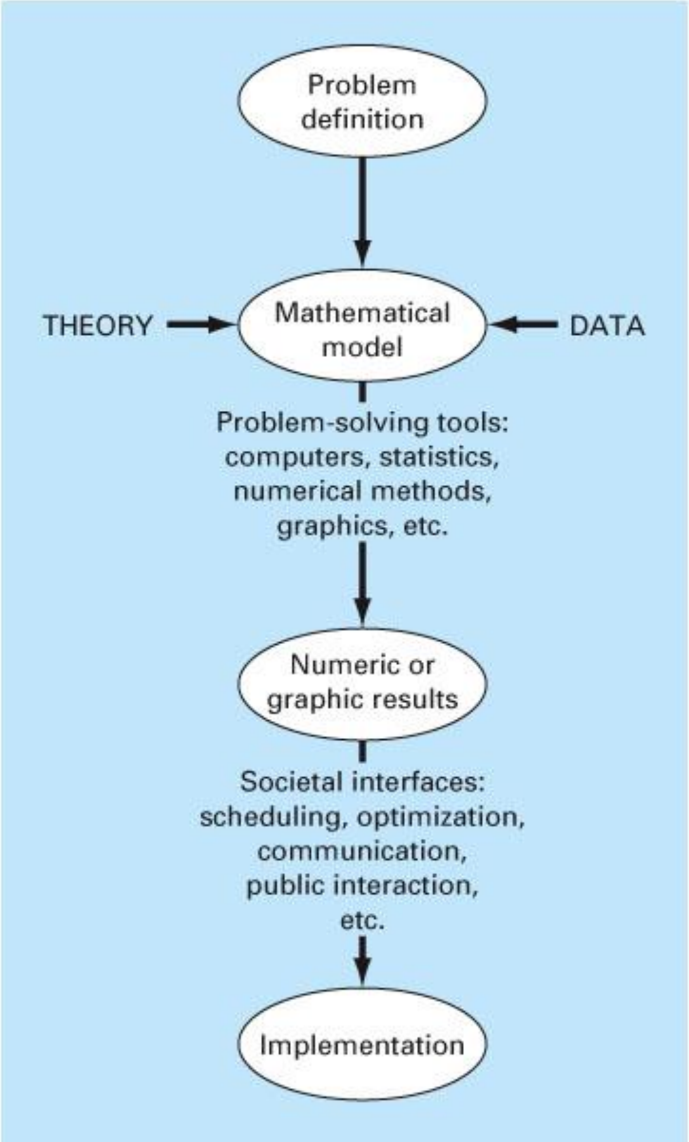
Taylor Series

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.



Problem solving process



Taylor's Theorem

Suppose $f \in C^n[a, b]$ and $f^{(n+1)}$ exists on [a, b]. Let x_0 be a number in [a, b]. For every x in [a, b], there exists a number $\xi(x)$ between x_0 and x with

$$f(x) = Pn(x) + Rn_{(x)}$$

where

$$P_n(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \cdots + \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k$$

And

$$R_n(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x - x_0)^{(n+1)}$$

$P_n(x)$ _ the n^th Taylor polynomial for f about x_0.

$R_n(x)$ _ the **truncation error** (or *remainder term*) associated with $P_n(x)$.

nth order approximation

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

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

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

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

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

Example

Determine

(a) the second and

(b) the third Taylor polynomials for $f(x) = \cos x$ about $x_0 = 0$, and use these polynomials to approximate $\cos(0.01)$.

(c) Use the third Taylor polynomial and its remainder term to approximate $\int_0^{0.1} cosx\, dx$.

Since $f \in C^\infty(IR)$, Taylor's Theorem can be applied for any $n \geq 0$. Also,

$$f'(x) = -\sin x,$$
$$f''(x) = -\cos x,$$
$$f'''(x) = \sin x, \text{ and}$$
$$f^{(4)}(x) = \cos x,$$

so

$$f(0) = 1,$$
$$f'(0) = 0,$$
$$f''(0) = -1, \text{ and}$$
$$f'''(0) = 0.$$

Example (cont)

a. For n = 2 and x_0 = 0, we have

$$cosx = f(0) + f'(0)x + \frac{f''(0)}{2!}x^2 + \frac{f'''(\xi(x))}{3!}x^3$$

$$= 1 - \frac{1}{2}x^2 + \frac{1}{6}x^3 \sin \xi(x)$$

When x=0.01, this becomes

$$\cos(0.01) = 1 - \frac{1}{2}(0.01)^2 + \frac{1}{6}(0.01)^3 \sin \xi(0.01)$$

$$= 0.99995 + \frac{10^{-6}}{6} \sin \xi(0.01)$$

$$E_t = |\cos(0.01) - 0.99995|$$

$$= 0.16 \times 10^{-6} \sin \xi(x) \leq 0.16 \times 10^{-6}$$

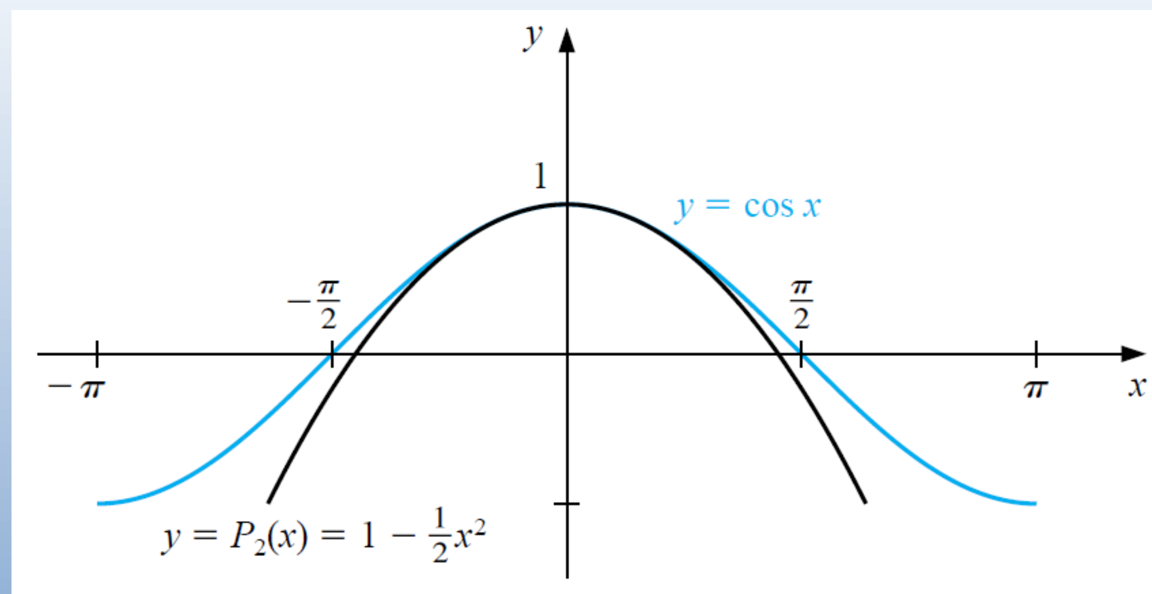
Example (cont)

b. For n = 3 and x_0 = 0, we have f'''(0)=0, the third Taylor polynomial and remainder term about x0 = 0 are

$$cosx = 1 - \frac{1}{2}x^2 + \frac{1}{24}x^4 \cos\xi(x) = 0.99995$$

and

$$\left|\frac{1}{24}x^4 \, cos\,\xi(0.01)\right| \leq \frac{1}{24}(0.01)^4(1) \approx 4.2 \times 10^{-10}$$



Example (cont)

c. Using the third Taylor polynomial gives

$$\int_0^{0.1} \cos x \, dx = \int_0^{0.1} \left(1 - \frac{1}{2}x^2\right) dx$$

$$+ \int_0^{0.1} \left(\frac{1}{24}x^4 \cos \xi(x)\right) dx$$

$$= \left[x - \frac{1}{6}x3\right]_0^{0.1} + \frac{1}{24}\int_0^{0.1} x^4 cosxdx$$

$$= 0.1 - \frac{1}{6}(0.1)^3 + \frac{1}{24}\int_0^{0.1} x^4 cosxdx$$

Therefore,

$$\int_0^{0.1} \cos x \, dx \approx 0.1 - \frac{1}{6}(0.1)^3 = 0.09983$$

So,

$$Et = \left|\sin x_0^{0.1} - 0.09983\right| \approx 8.4 \times 10^{-8}$$

Example

Suppose we want the Taylor series at 0 of the function

$$g(x) = \frac{e^x}{\cos x}.$$

We have for the exponential function

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \cdots$$

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

Assume the power series is

$$\frac{e^x}{\cos x} = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + \cdots$$

Then multiplication with the denominator and substitution of the series of the cosine yields

$$\begin{aligned} e^x &= (c_0 + c_1 x + c_2 x^2 + c_3 x^3 + \cdots) \cos x \\ &= \left(c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4 + \cdots\right) \left(1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \cdots\right) \\ &= c_0 - \frac{c_0}{2} x^2 + \frac{c_0}{4!} x^4 + c_1 x - \frac{c_1}{2} x^3 + \frac{c_1}{4!} x^5 + c_2 x^2 - \frac{c_2}{2} x^4 + \frac{c_2}{4!} x^6 + c_3 x^3 - \end{aligned}$$

Example (cont)

Collecting the terms up to fourth order yields

$$= c_0 + c_1 x + \left(c_2 - \frac{c_0}{2}\right) x^2 + \left(c_3 - \frac{c_1}{2}\right) x^3 + \left(c_4 - \frac{c_2}{2} + \frac{c_0}{4!}\right) x^4 + \cdots$$

Comparing coefficients with the above series of the exponential function yields the desired Taylor series

$$\frac{e^x}{\cos x} = 1 + x + x^2 + \frac{2x^3}{3} + \frac{x^4}{2} + \cdots.$$

Taylor series in several variables

For a function that depends on two variables, x and y, the Taylor series to second order about the point (a, b) is

$$f(a,b) + (x-a)\,f_x(a,b) + (y-b)\,f_y(a,b) \\ \qquad + \frac{1}{2!}\left[(x-a)^2\,f_{xx}(a,b) + 2(x-a)(y-b)\,f_{xy}(a,b) + (y-b)^2\,f_{yy}(a,b)\right]$$

where the subscripts denote the respective partial derivatives.

Example

Compute a second-order Taylor series expansion around point (a, b) = (0, 0) of a function

$$f(x,y) = e^x \log(1+y).$$

Firstly, we compute all partial derivatives we need

$$f_x(a,b) = e^x \log(1+y)\Big|_{(x,y)=(0,0)} = 0\,,$$

$$f_y(a,b) = \frac{e^x}{1+y}\Big|_{(x,y)=(0,0)} = 1\,,$$

$$f_{xx}(a,b) = e^x \log(1+y)\Big|_{(x,y)=(0,0)} = 0\,,$$

$$f_{yy}(a,b) = -\frac{e^x}{(1+y)^2}\Big|_{(x,y)=(0,0)} = -1\,,$$

$$f_{xy}(a,b) = f_{yx}(a,b) = \frac{e^x}{1+y}\Big|_{(x,y)=(0,0)} = 1.$$

The Taylor series is

$$T(x,y) = f(a,b) + (x-a)\,f_x(a,b) + (y-b)\,f_y(a,b) + \frac{1}{2!}\left[(x-a)^2\,f_{xx}(a,b) + 2(x-a)(y-b)\,f_{xy}(a,b) + (y-b)^2\,f_{yy}(a,b)\right] + \cdots,$$

$$T(x,y) = 0 + 0(x-0) + 1(y-0) + \frac{1}{2}\Big[0(x-0)^2 + 2(x-0)(y-0) + (-1)(y-0)^2\Big] + \cdots$$

$$= y + xy - \frac{y^2}{2} + \cdots\,.$$

PART C

OTHER APPLICATIONS OF TAYLOR’S SERIES

Numerical Differentiation

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

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

- First Forward Difference

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i) + R_1$$

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

- First Backward Difference

$$f(x_{i-1}) \cong f(x_i) - f'(x_i)(x_i - x_{i-1}) + R_1$$

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

Numerical Differentiation

- First Centered Difference

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)h + R_1$$

$$f(x_{i-1}) \cong f(x_i) - f'(x_i)h + R_1$$

$$f(x_i) \cong f(x_{i-1}) + f'(x_i)h + R_1$$

$$=> f(x_{i+1}) \cong f(x_{i-1}) + 2f'(x_i)h + R_1$$

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

Example

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

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

$x_{i-1} = 0$

$x_i = 0.5$

$x_{i+1} = 1.0$

$f(x_{i-1}) = 1.2$

$f(x_i\ ) = 0.925$

$f(x_{i+1}) = 0.2$

These values can be used to compute the forward divided difference

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

Example

The backward divided difference

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

And the centered divided difference

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

Example

2. For h = 0.25, the function can be employed to determine

$x_{i-1} = 0.25$

$x_i = 0.5$

$x_{i+1} = 0.75$

$f(x_{i-1}) = 1.10351563$

$f(x_i) = 0.925$

$f(x_{i+1}) = 0.63632813$

These values can be used to compute the forward divided difference

$$f'(0.5) = \frac{0.63632813 - 0.925}{0.25} = -1.155$$

$$|\varepsilon_t| = 26.5\%$$

Example

The backward divided difference

$$f'(0.5) = \frac{0.925 - 1.10351563}{0.25} = -0.714$$

$$|\varepsilon_t| = 21.7\%$$

And the centered divided difference

$$f'(0.5) = \frac{0.63632813 - 1.10351563}{0.5} = -0.934$$

$$|\varepsilon_t| = 2.4\%$$

Finite Difference Approximation of Higher Derivatives

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

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

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

$$=> f(x_{i+2}) - 2f(x_{i+1}) \cong -f(x_i) + f''(x_i)h^2 + \ldots$$

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

Error Propagation

Function of a Single Variable

Suppose that we have a function $f\,(x)$ that is dependent on a single independent variable x. Assume that $\bar{x}$ is an approximation of x. We, therefore, would like to assess the effect of the discrepancy between x and $\bar{x}$ on the value of the function. That is, we would like to estimate

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

where

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

$$f(x) - f(\bar{x}) = f'(\bar{x})(x - \bar{x})$$

or

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

Example

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

We have $\Delta f(\bar{x}) = |f'(\bar{x})|\Delta\bar{x}$, so

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

Because f(2.5)=15.625, we predict that

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

Error Propagation

Function of More than One Variable

For n independent variables $\overline{x_1}$, $\overline{x_2}$, ..., $\overline{x_n}$ having errors $\Delta\overline{x_1}$, $\Delta\overline{x_2}$,..., $\Delta\overline{x_n}$, the following general relationship holds:

$$\Delta f(\overline{x_1}, \overline{x_2}, ..., \overline{x_n}) \cong \left|\frac{\partial f}{x_1}\right| \Delta\overline{x_1} + \left|\frac{\partial f}{x_2}\right| \Delta\overline{x_2} + ... + \left|\frac{\partial f}{x_n}\right| \Delta\overline{x_n}$$

Summary

Error Definitions

True error	$E_t = \text{true value} - \text{approximation}$
True percent relative error	$\varepsilon_t = \dfrac{\text{true value} - \text{approximation}}{\text{true value}}\, 100\%$
Approximate percent relative error	$\varepsilon_a = \dfrac{\text{present approximation} - \text{previous approximation}}{\text{present approximation}}\, 100\%$
Stopping criterion	Terminate computation when $\varepsilon_a < \varepsilon_s$ where ε_s is the desired percent relative error

Taylor Series

Taylor series expansion	$f(x_{i+1}) = f(x_i) + f'(x_i)h + \dfrac{f''(x_i)}{2!}h^2 + \dfrac{f'''(x_i)}{3!}h^3 + \cdots + \dfrac{f^{(n)}(x_i)}{n!}h^n + R_n$ where
Remainder	$R_n = \dfrac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1}$ or $R_n = O(h^{n+1})$

Any Questions?

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