# SKTN 2393
# Numerical Methods for Nuclear Engineers

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# Solve this!

$$\frac{dy}{dx} = (x - 1)^3$$

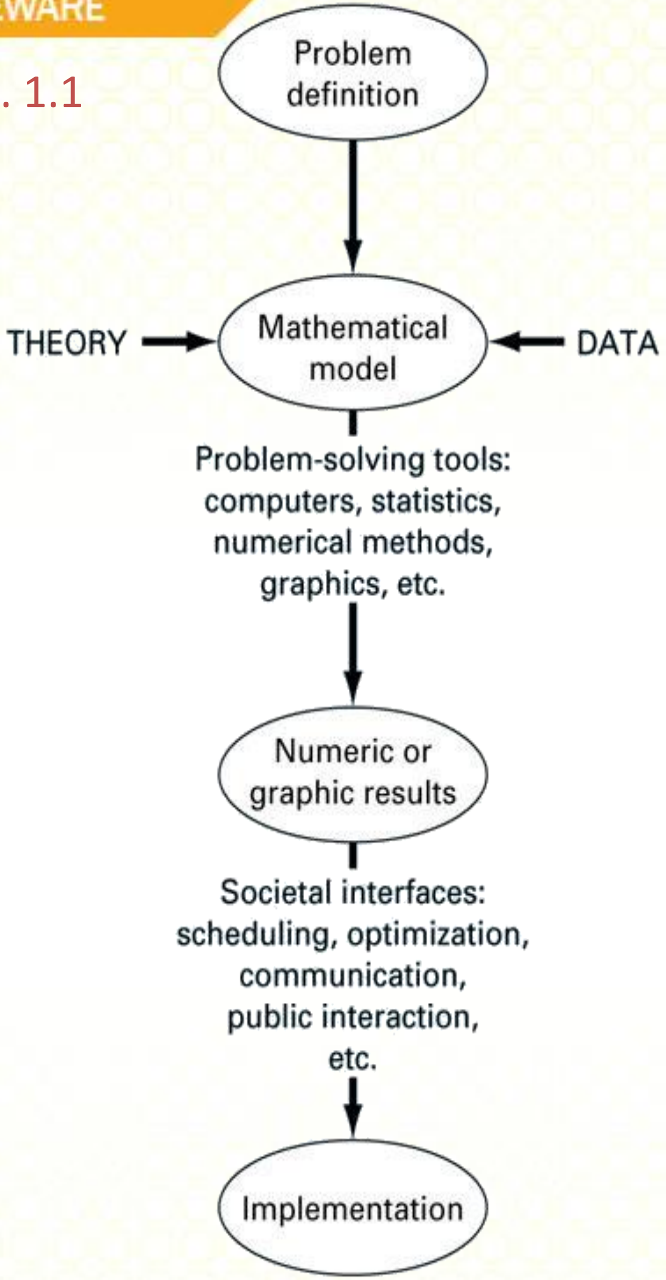
Given that

$$y(0) = 2$$

# Solving Engineering Problems

- From physical problem to solution
  - Develop Model
  - Apply Fundamental Principles
  - Obtain Governing Equations
  - Solution of Governing Equations
  - Interpretation of Solution

Fig. 1.1

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- A mathematical model is represented as a functional relationship of the form

$$\text{Dependent Variable} = f\left(\text{independent variables},\ \text{parameters},\ \text{forcing functions}\right)$$

- *Dependent variable*: Characteristic that usually reflects the state of the system
- *Independent variables*: Dimensions such as time ans space along which the systems behavior is being determined
- *Parameters*: reflect the system's properties or composition
- *Forcing functions*: external influences acting upon the system

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# Falling Parachutist Problem

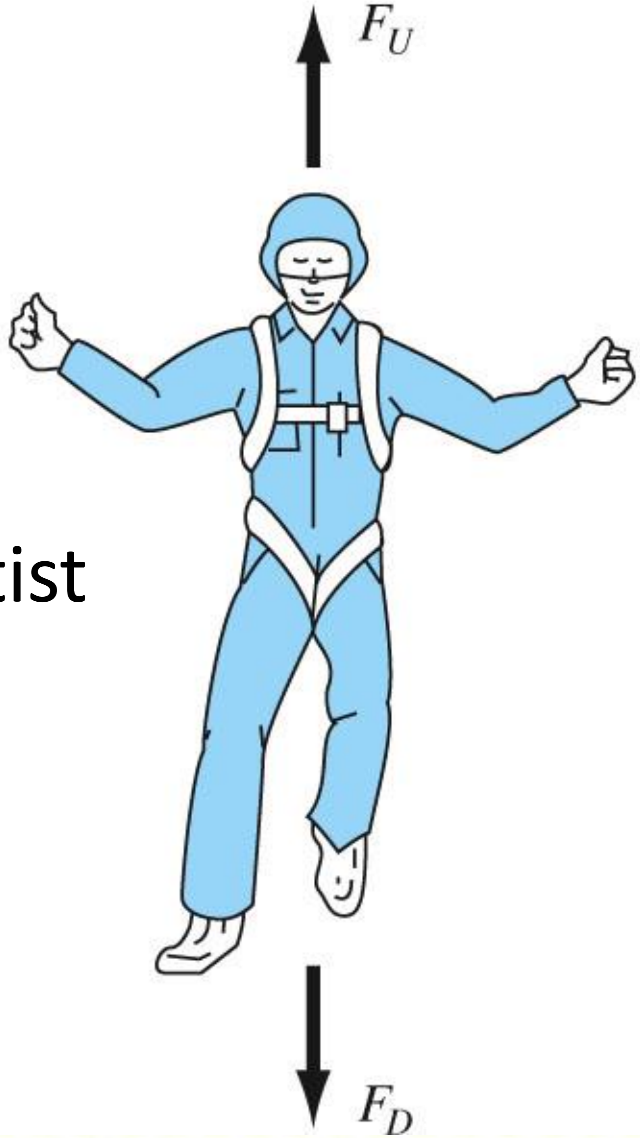


Figure 1_02.jpg

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# Develop Model

- Model is developed to represent all important characteristics of the physical system
  - Identify system
  - Identify external influences on system (load, input, output)
  - Material properties (Ideal gas, real gas, Newtonian fluid, Elastic/plastic etc.)

# Apply Fundamental Principles

- Apply Physical Laws
  - Equilibrium equation
  - Newton's Law of motion
  - Conservation of mass
  - Conservation of momentum
  - Conservation of energy
  - Accounting principle (change = input - output)

$$\frac{dv}{dt} = \frac{F}{m}$$

$$F = F_D + F_U$$

$$F_D = mg$$

$$F_U = -cv$$

$$\frac{dv}{dt} = \frac{mg - cv}{m}$$

# Obtain governing equation

- Apply simplifying assumptions on the physical laws
- Derive final governing equation

$$\frac{dv}{dt} = g - \frac{c}{m}v$$

- This is a differential equation and is written in terms of the differential rate of change dv/dt of the variable that we are interested in predicting.
- If the parachutist is initially at rest (v=0 at t=0), using calculus

Independent variable

$$v(t) = \frac{gm}{c}\left(1 - e^{-(c/m)t}\right)$$

Dependent variable

Forcing function

Parameters

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# Solution of governing equation

- The problem may now appear mathematically as a set of
  - linear/nonlinear algebraic equations
  - Transcendental equations
  - Ordinary differential equations (ODE)
  - Partial differential equations (PDE)
  - Eigenvalue problem
- The set of simultaneous equations is readily handled using matrices.

# Solutions of governing equations

- Two types of solutions
  - Closed form mathematical expression leading to analytical solution
  - Closed form not possible, thus needs approximated numerical solution (computers)
- This is the "big picture" of this course.

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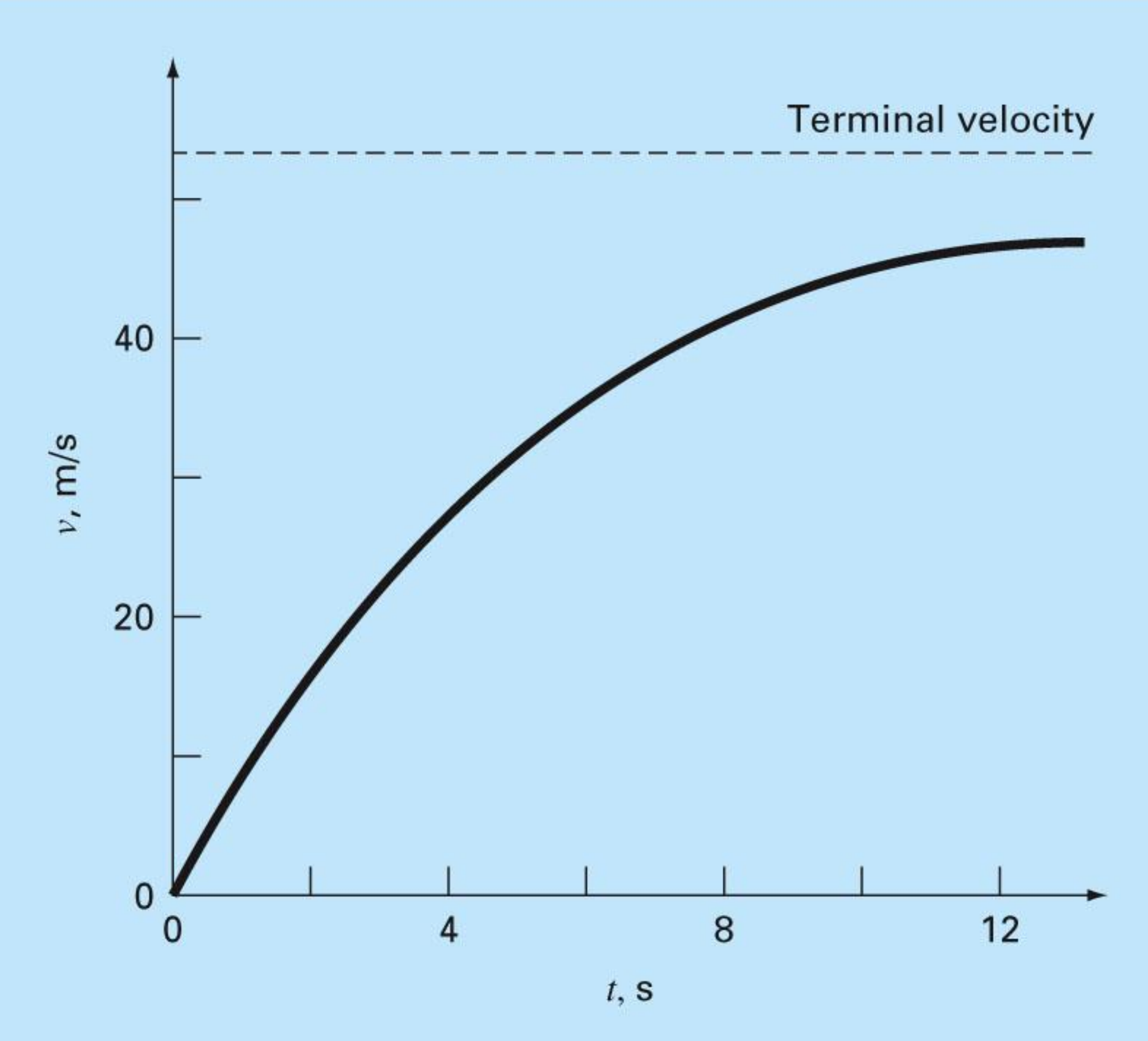

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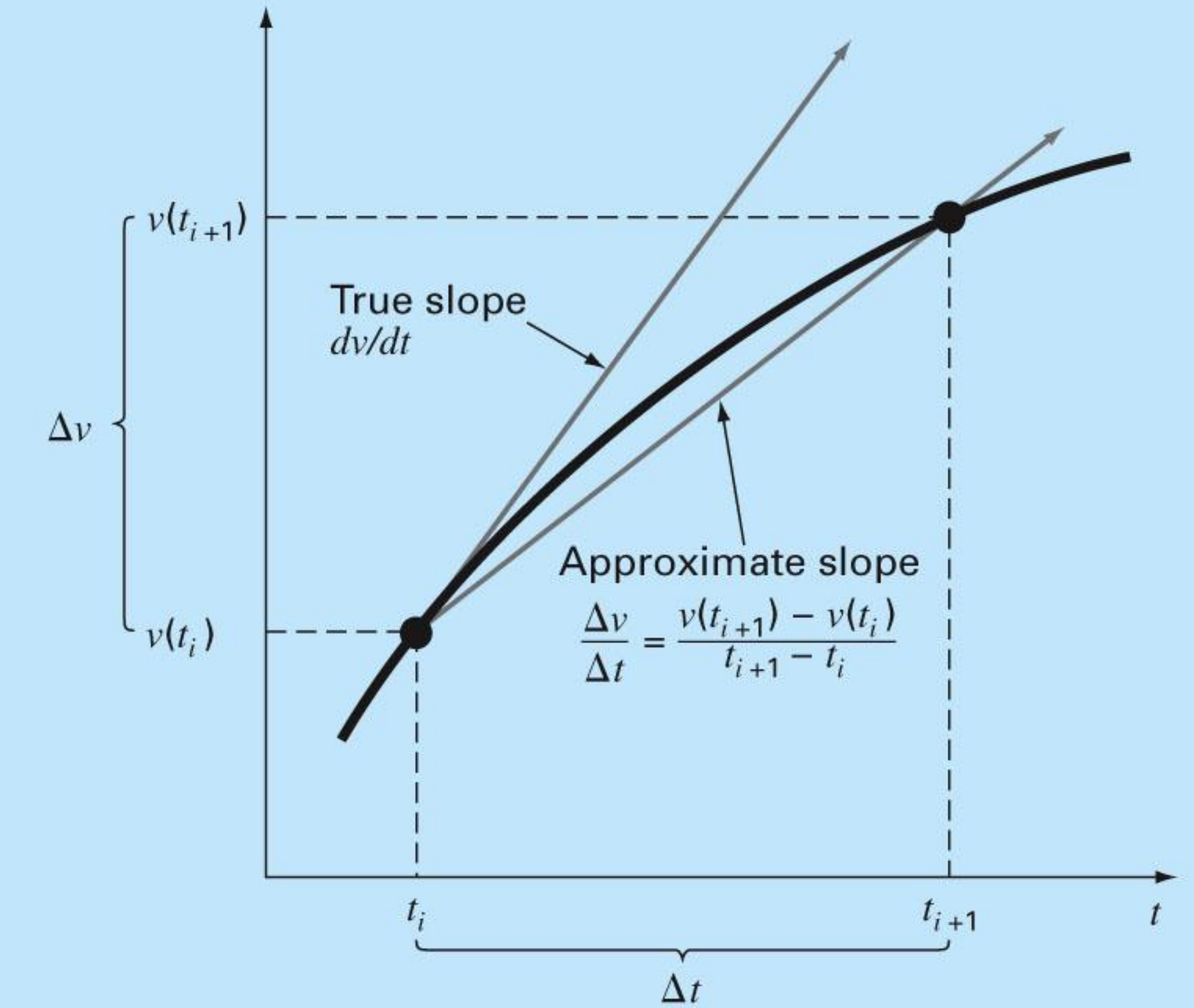

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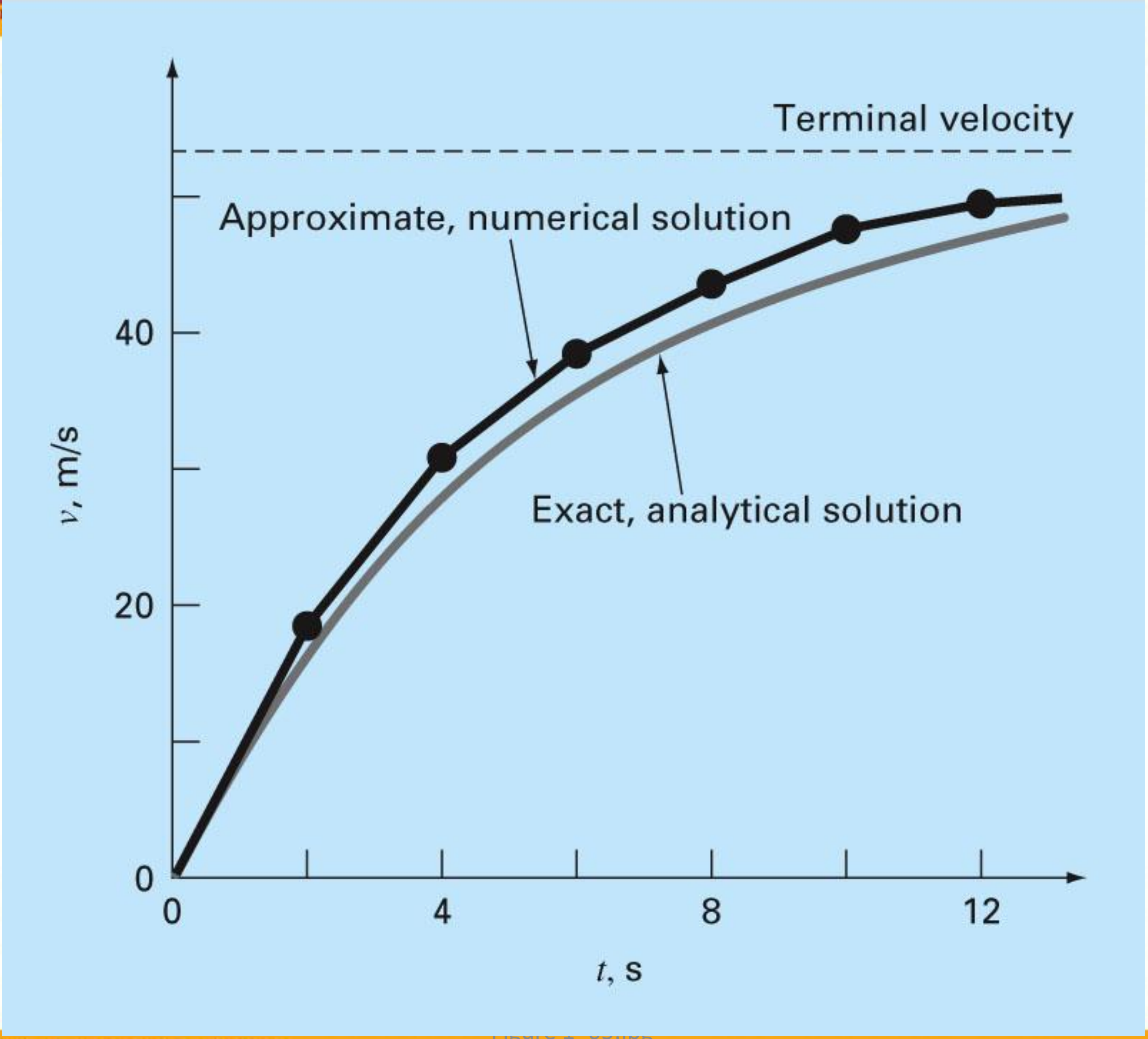


Figure 1_03.jpg

# Solution of governing equation

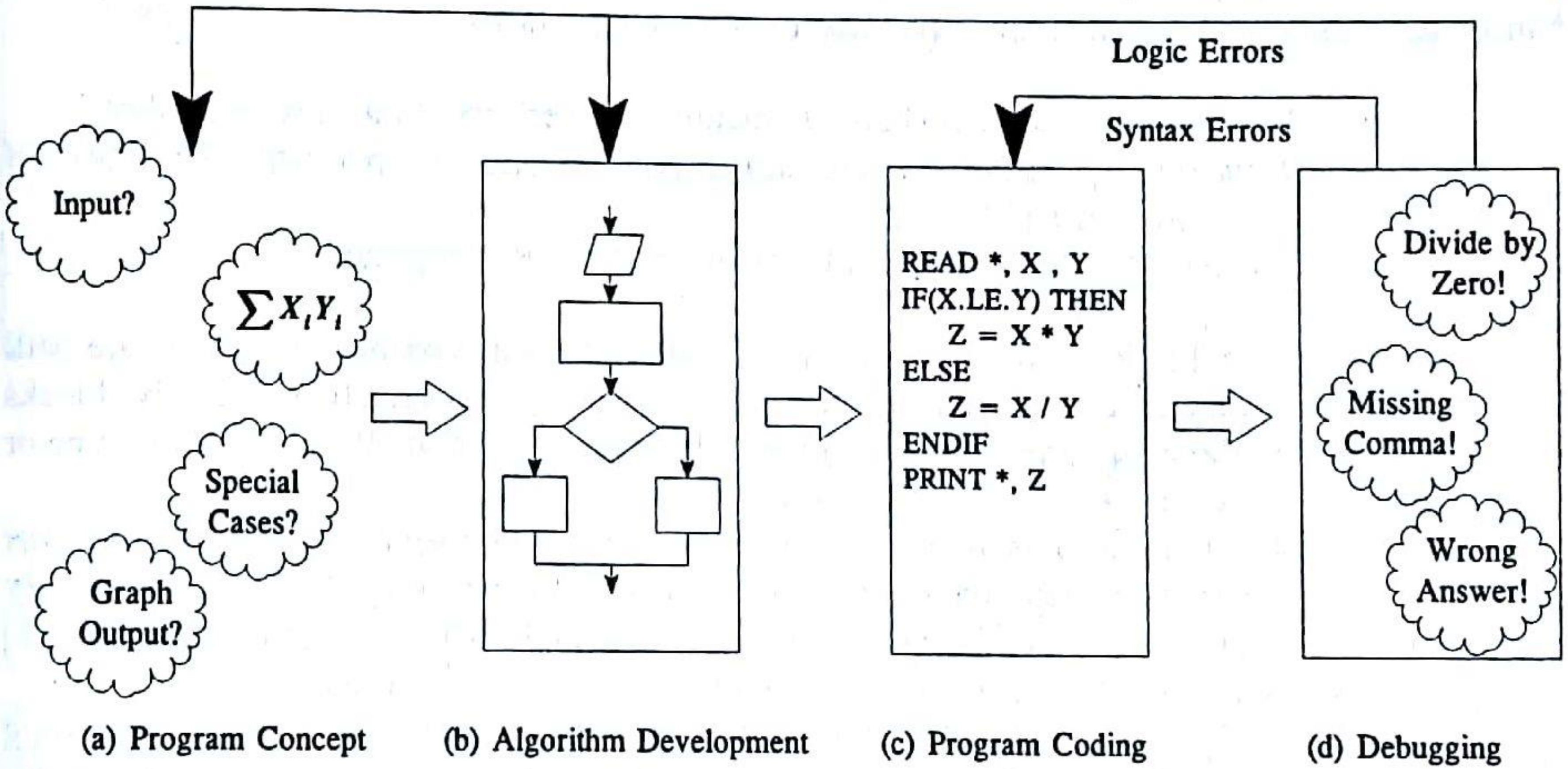


**Fig. 1-1 Stages of program development**

# Interpretation of Solution

- Reality Check
  - Test with simple, known cases
- Graphics representation better conveys the meaning of solution
  - Graphs
  - Bar charts
  - Contour plots

# Verification (Reality Check)

- In some engineering work, actual physical experiments must be carried out to verify one's findings.
- Starting today, get into the habit of asking yourself if your solution to a problem makes sense.
- Asking your instructor if you have come up with the right answer or checking the back of your textbook to match answers are not good approaches in the long run.
- You need to develop the means to check your results by asking yourself the appropriate questions.
- Remember, once you start working for hire, there are no answer books. You will not want to run to your boss to ask if you did the problem right!

# Softwares

- Languages
  - FORTRAN
  - Matlab
  - C, C++, Python, etc
- Libraries
  - Netlib (www.netlib.org)
  - LAPACK
  - EISPACK
  - LINPACK
  - IMSL, etc

# Softwares

- Others
- Octave, Scilab
- Maxima, Maple
- Mathematica, Mathcad
- R (statistical)
- OpenDX, Paraview, Viz5D (plotting, visualization)

# 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.

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# Taylor Series

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

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

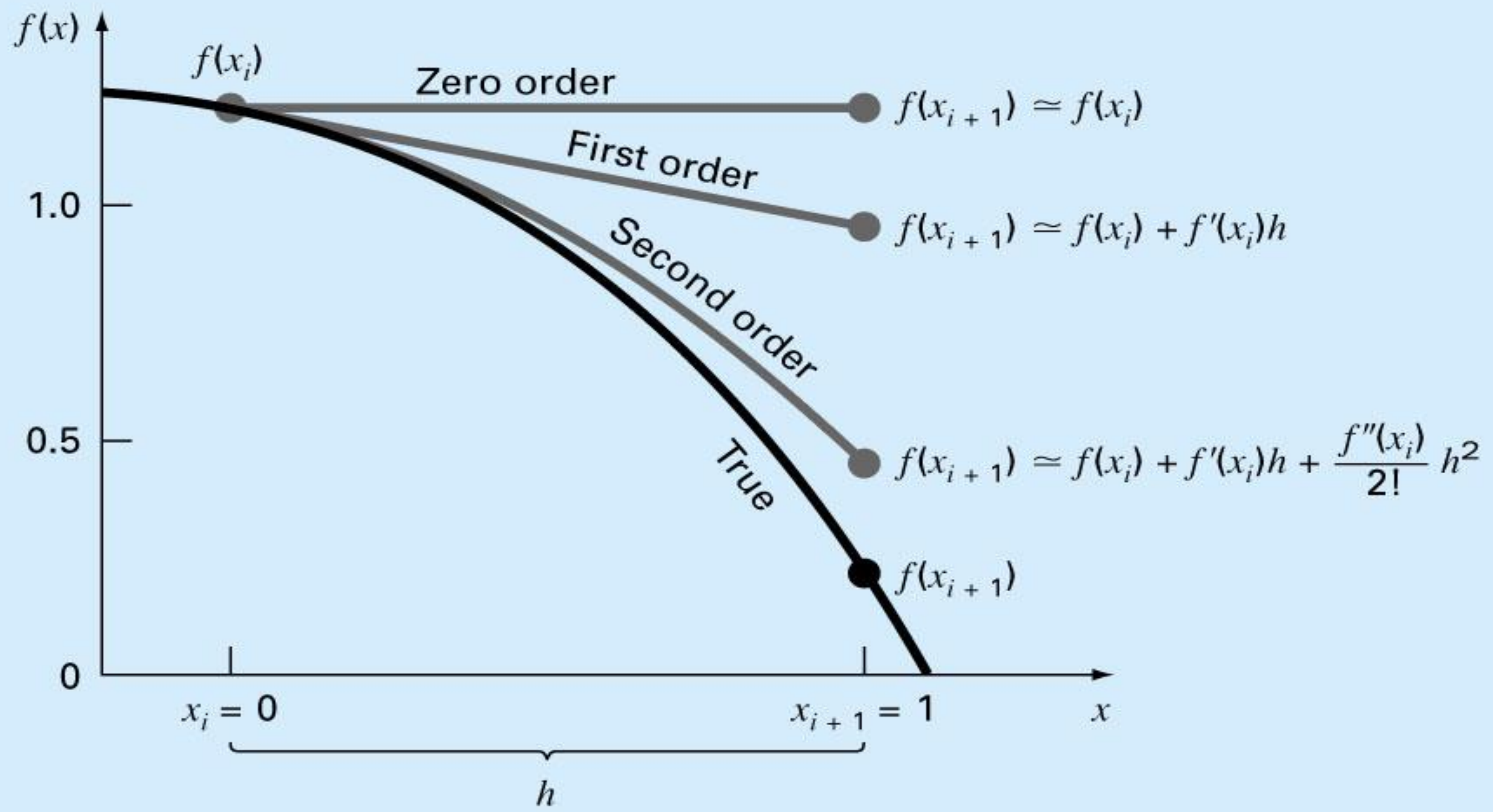
$$R_n = \frac{f^{(n+1)}(\varepsilon)}{(n+1)!} h^{(n+1)}$$

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

- Any smooth function can be approximated as a polynomial.

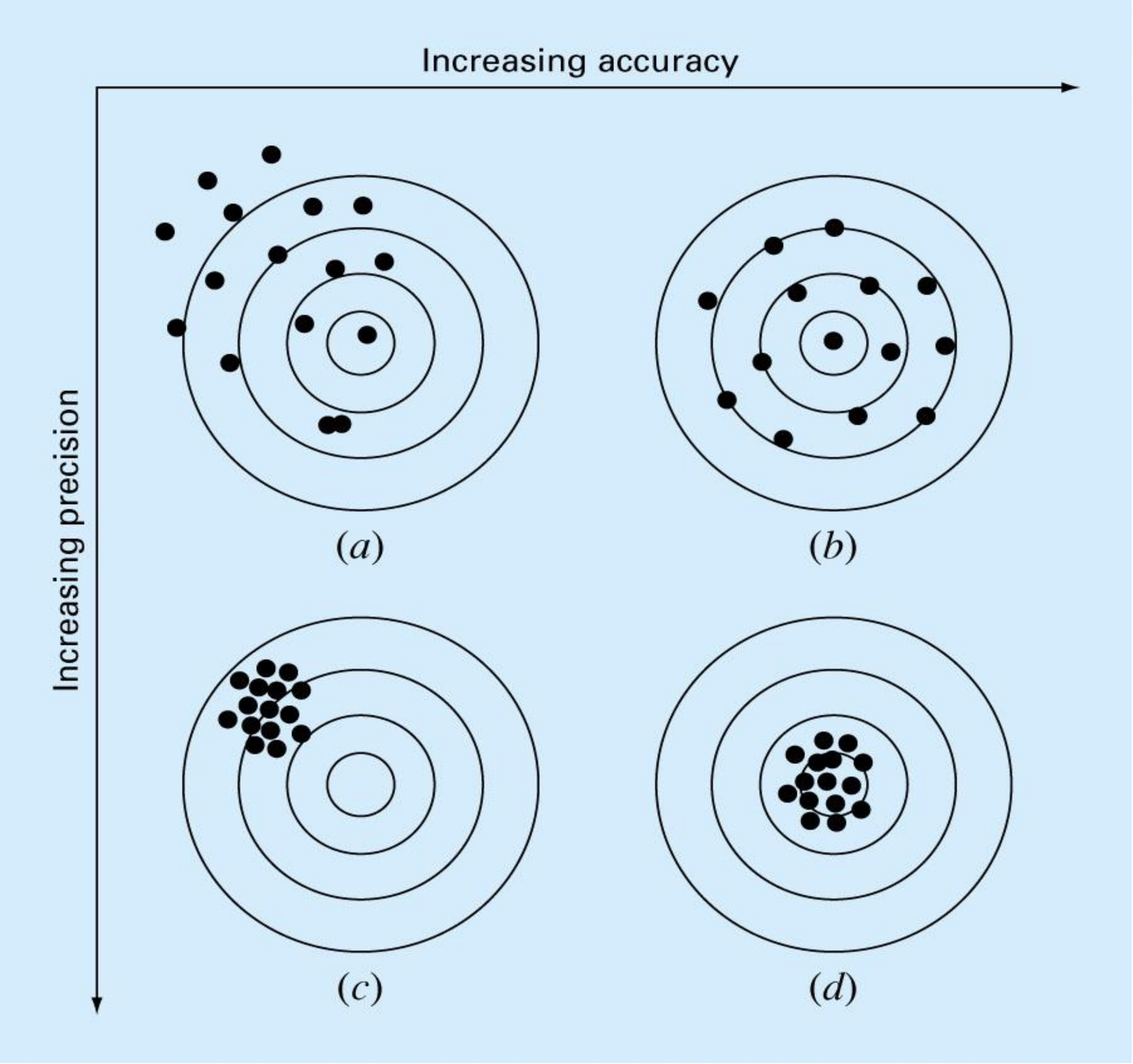
$f(x_{i+1}) \approx f(x_i)$ *zero order* approximation, only true if $x_{i+1}$ and $x_i$ are very close to each other.

$f(x_{i+1}) \approx f(x_i) + f'(x_i)(x_{i+1}-x_i)$ *first order* approximation, in form of a straight line


$f(x)$
$f(x_i)$
Zero order
$f(x_{i+1}) \simeq f(x_i)$
First order
$f(x_{i+1}) \simeq f(x_i) + f'(x_i)h$
Second order
$f(x_{i+1}) \simeq f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2$
True
$f(x_{i+1})$
1.0
0.5
0
$x_i = 0$
$x_{i+1} = 1$
$x$
$h$

# Precision and Accuracy

- Accuracy. How close is a computed or measured value to the true value
- Precision (or *reproducibility*). How close is a computed or measured value to previously computed or measured values.
- Inaccuracy (or *bias*). A systematic deviation from the actual value.
- Imprecision (or *uncertainty*). Magnitude of scatter.

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# Errors

- For many engineering problems, we cannot obtain analytical solutions.
- Numerical methods yield approximate results, results that are close to the exact analytical solution. We cannot exactly compute the errors associated with numerical methods.
  - Only rarely given data are exact, since they originate from measurements. Therefore there is probably error in the input information.
  - Algorithm itself usually introduces errors as well, e.g., unavoidable round-offs, etc …
  - The output information will then contain error from both of these sources.
- How confident we are in our approximate result?
- The question is "*how much error is present in our calculation and is it tolerable?*"

# Errors

- Types
  - Absolute
  - Relative

# Error Definitions

True Value = Approximation + Error

$E_t$ = True value – Approximation (+/-)

True error (**<u>Absolute Error</u>**)

$$\text{True fractional relative error} = \frac{\text{true error}}{\text{true value}}$$

$$\text{True percent }\underline{\text{relative error}},\ \varepsilon_t = \frac{\text{true error}}{\text{true value}} \times 100\%$$

# Errors

- True or Absolute Error

$$E_x = x - \tilde{x}$$

- Relative Error

$$R_x = \frac{x - \tilde{x}}{x}, \qquad x \neq 0$$

- $x =$ true value, $\tilde{x} =$ approximate value

# In Absence of True Value

- For numerical methods, the true value will be known only when we deal with functions that can be solved analytically (simple systems). In real world applications, we usually do not know the answer a priori. Then

$$\varepsilon_{\mathrm{a}} = \frac{\text{Approximate error}}{\text{Approximation}} \times 100\%$$

- *Iterative approach,* example Newton's method

$$\varepsilon_{\mathrm{a}} = \frac{\text{Current approximation - Previous approximation}}{\text{Current approximation}} \times 100\%$$

(+ / -)

# Tolerance

- Use absolute value.
- Computations are repeated until stopping criterion is satisfied.

$$|\varepsilon_a| < \varepsilon_s$$

Pre-specified % tolerance based on the knowledge of your solution

- If the following criterion is met

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

you can be sure that the result is correct to at least <u>n significant</u> figures.

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# Error (Example Problem)

**Problem Statement:**
Suppose that you are asked to measure the lengths of a bridge and a rivet, and came up with 9,999 cm and 9 cm, respectively. If the true values are 10,000 cm and 10 cm, respectively, compute the *absolute* error and the r*elative* error (in %) for each case.

**Solution:**
Absolute error for measuring
bridge: $E_x = x - \tilde{x} = 10000 - 9999 =$ 1 cm
rivet: $E_x = x - \tilde{x} = 10 - 9 =$ 1 cm

Percent relative error for measuring
bridge: $R_x = \frac{x-\tilde{x}}{x} \times 100 = 0.01\%$
rivet: $R_x = \frac{x-\tilde{x}}{x} \times 100 = 10\%$

# Sources of Error

- Errors in mathematical modeling:
  - simplifying approximation,
  - assumption made in representing physical system by mathematical equations
- Blunders:
  - undetected programming errors,
  - silly mistakes
- Errors in input:
  - due to unavoidable reasons e.g. errors in data transfer,
  - uncertainties associated with measurements

# Sources of Error

- Machine errors:
  - rounding,
  - chopping,
  - overflow,
  - underflow
- Truncation errors associated with mathematical process:
  - approximate evaluation of an infinite series,
  - integral involving infinity

# Round-off Errors

- Numbers such as π, 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

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

exponent

mantissa

Base of the number system used

# Chopping

Example:

$\pi$=3.14159265358 to be stored on a base-10 system carrying 7 significant digits.

$\pi$=3.141592 chopping error $\varepsilon_t$=0.00000065

If rounded

$\pi$=3.141593 $\varepsilon_t$=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.

# Error Propagation

- All of the errors can accumulate and be propagated to the final result producing uncertainties.
- Error in the output of a procedure due to the error in the input data
- Output of a procedure $f$ is a function of input parameters $(x_1, x_2, \dots, x_n)$

$$f = f(x_1, x_2, \cdots x_n) \equiv f(\vec{X})$$

# Error Propagation

- Value of $f$ is found by Taylor's series expansion about the approximate values $\vec{X} = \{\bar{x}_1, \bar{x}_2, \cdots, \bar{x}_n\}^T$

$$
\begin{aligned}
f(x_1, x_2, \cdots x_n) = \quad & f(\bar{x}_1, \bar{x}_2, \cdots, \bar{x}_n) + \frac{\partial f}{\partial x_1}\left(\bar{\vec{X}}\right)(x_1 - \bar{x}_1) \\
& + \frac{\partial f}{\partial x_2}\left(\bar{\vec{X}}\right)(x_2 - \bar{x}_2) + \cdots \\
& + \frac{\partial f}{\partial x_n}\left(\bar{\vec{X}}\right)(x_n - \bar{x}_n) + \\
& \text{higher order derivative terms}
\end{aligned}
$$

# Error Propagation

- Neglecting higher order derivative terms, the error in the output can be expressed as

$$\Delta f = f - \bar{f}$$
$$\equiv f(x_1, x_2, \ldots, x_n) - f(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n)$$

and denoting errors in input parameters as

$$\Delta x_i = x_i - \bar{x}_i, \quad i = 1, 2, \ldots, n$$

we can estimate propagation error as

$$\Delta f \approx \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(\bar{\vec{X}})(x_i - \bar{x}_i)$$

# Error Propagation

- If $f(x_1, x_2, \cdots x_n) \neq 0$ and $x_i \neq 0$, the relative propagation error, $\varepsilon_f$ is

$$\varepsilon_f = \frac{\Delta f}{f} = \sum_{i=1}^{n} \left\{ \frac{x_i}{f(\vec{X})} \frac{\partial f}{\partial x_i}(\vec{\bar{X}}) \right\} \varepsilon_{x_i}$$

where $\varepsilon_{x_i}$ is

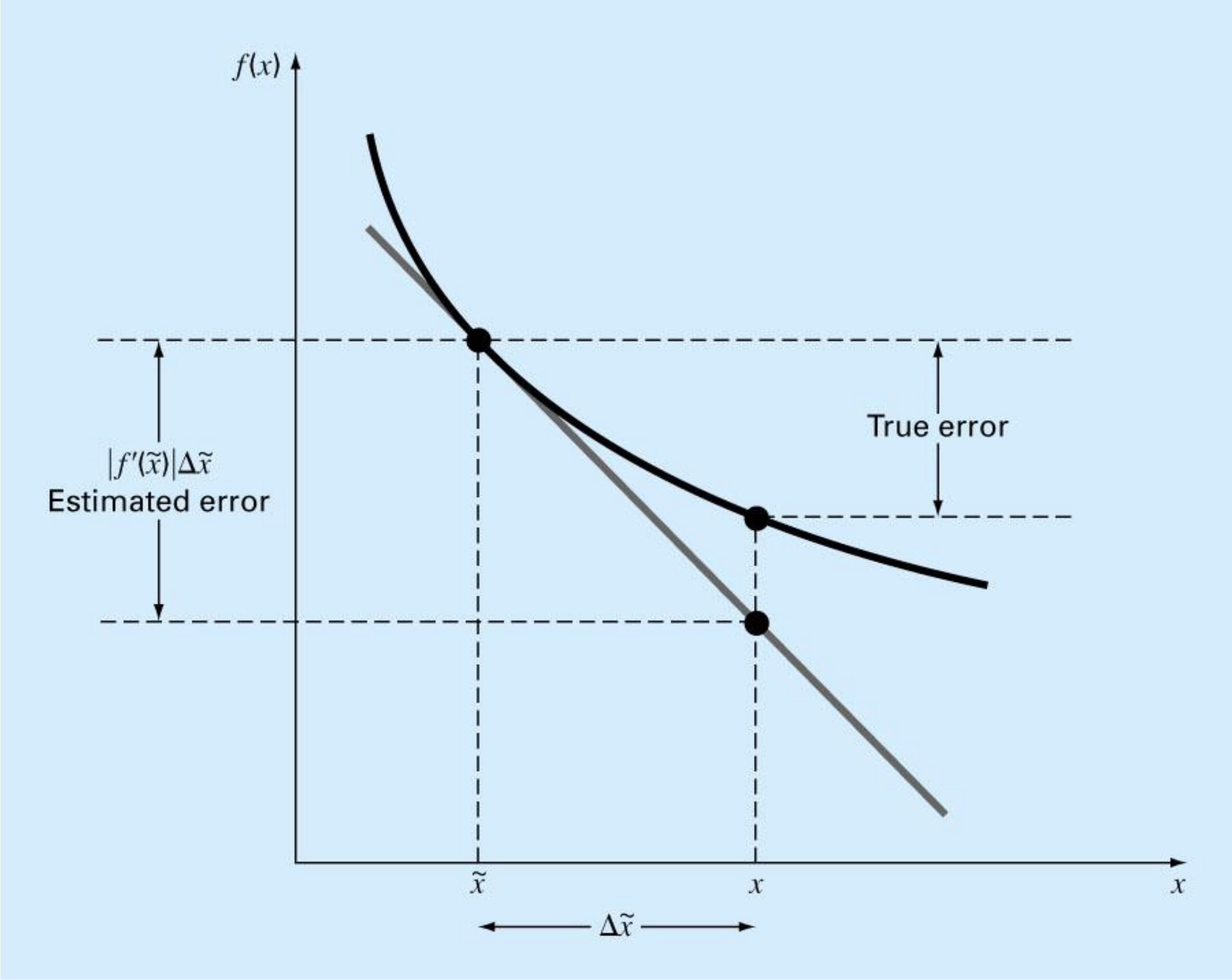
$$\varepsilon_{x_i} = \frac{x_i - \bar{x}_i}{x_i} \quad i = 1, 2, \ldots, n$$

- The quantity

$$c_i = \left\{ \frac{x_i}{f(\vec{X})} \frac{\partial f}{\partial x_i}(\vec{\bar{X}}) \right\}$$

is called the amplification or condition number of relative input error $\varepsilon_{x_i}$

# Error Propagation



# Propagation of Error (Example)

**Problem Statement:**

The deflection $y$ of the top of a sailboat mast is

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

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

$$F = 50 \text{ lb/ft} \qquad L = 30 \text{ ft} \qquad E = 1.5 \times 10^8 \text{ lb/ft}^2 \qquad I = 0.06 \text{ ft}^4$$

$$\Delta F = 2 \text{ lb/ft} \qquad \Delta L = 0.1 \text{ ft} \qquad \Delta E = 0.01 \times 10^8 \text{ lb/ft}^2 \qquad \Delta I = 0.0006 \text{ ft}^4$$

**Solution:**

Work through the example.

# Propagation of Error (Arithmetic Operation)

- When two numbers are used in an arithmetic operations, the numbers cannot be stored exactly by the floating-point representation.
- Let $x$ and $y$ be the exact number and $\tilde{x}$ and $\tilde{y}$ their approximate values. Then

$$x = \tilde{x} + \varepsilon_x \qquad\qquad y = \tilde{y} + \varepsilon_y$$

$\varepsilon_x$ and $\varepsilon_y$ denote errors in $x$ and $y$, respectively.

- When arithmetic operation, say multiplication, is carried out on the numbers, associated error, $E$, results

$$E = xy - \tilde{x}\tilde{y} = xy - (x - \varepsilon_x)(y - \varepsilon_y) = x\varepsilon_y + y\varepsilon_x - \varepsilon_x\varepsilon_y$$

and relative error, $R$, is

$$R = \frac{E}{xy} = \frac{\varepsilon_x}{x} + \frac{\varepsilon_y}{y} - \frac{\varepsilon_x}{x}\frac{\varepsilon_y}{y} = R_x + R_y - R_xR_y \approx R_x + R_y$$

where $|R_x| << 1$ and $|R_y| << 1$