Chapter 1: Mathematical Preliminaries

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教材、辅助教材与考试考核方法

- **教材:** Numerical Analysis(7th or 9th), Richard L. Burden,J. Douglas Faires,BROOKS/COLE,2010.
- **参考书:**
  1. 数值方法：MATLAB版（原书第四版），[美] Mathews, J.H., Fink, K.D.; 周璐等译，北京：电子工业出版社，2010.
  2. 数值计算引论(第2版)，白峰杉，高等教育出版社，2010年
  3. 数值分析（原书第2版）,[美] Timothy Sauer 著；裴玉茹，马赓宇译, 机械工业出版社,2014年
  4. Numerical Recipes in C++，PRESS, WILLIAM H. TEUKOLSKY, SAUL A. VETTERLING, WILLIAM T. FLANNERY, BRIAN P,CAMBRIDGE UNIV PRESS,2005.
  5. Scientific Computing: An Introductory Survey, Second Edition，McGraw-Hill,2002, 清华大学出版社出版影印发行
- **成绩计算:** 理论推导证明和数值实验报告（电子版提交）（50%）+期末闭卷考试(50%)

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What is Scientific Computing?

- **Equivalent description**
  - **Numerical analysis**
  - **Numerical Methods**
  - **Computational Methods**
  - **Numerical Mathematics**
  - **Numerical Computing**
  - **Scientific Computing** etc.

Main Contents:

1. **Methods** using computer to solve **mathematical problems** in science and engineering, which mostly are **continuous**.
2. **design and analysis of algorithms** for different mathematical problems.
3. **Theory and Application** of Numerical Approximation Techniques

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Why do we need to learn Scientific Computing methods?

- **Many mathematical problems** arising in the science and engineering, such as derivatives, integrals, nonlinearities, Linear Algebra problems, differential equations, etc. are **difficult to solve**.
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Features of Scientific Computing:

- Deals continuous quantities with numerical approximate techniques;
- Considers **effects** of approximations, such as **error**, **convergence**, **uniqueness**, **existence**.
- **Assessment** on algorithm: **efficiency**, **reliability**, **accuracy**, etc.

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What does this book concern?

- **Approximation Methods** for solving equation(s);
- **Polynomial and interpolation approximation**;
- **Numerical Differentiation and Integration**.
- **Numerical methods for ODE or PDE**
- **Eigenvalues and Eigenvectors**...

Steps for solving Mathematical Problems in computational simulations

1. **Mathematical modelling**, usually equations.
2. **Design algorithms** to solve these equations.
3. Implement algorithms in computer software.
4. **Run the software**
5. **Represent** the computed results in forms or graphical visualization.
6. **Interpret and validate**(解释和验证) the computed results.

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Definition 1.1 Limit of a function(函数的极限)

Let f be a function defined on a set X of real numbers. Then f has the **limit L** at x_o, written

$$\lim_{x \to x_o} f(x) = L,$$

if, given any real number $\varepsilon > 0$, there exists a real number $\delta > 0$ such that

$$|f(x) - L| < \varepsilon$$

whenever $x \in X$ and $0 < |x - x_o| < \delta$.

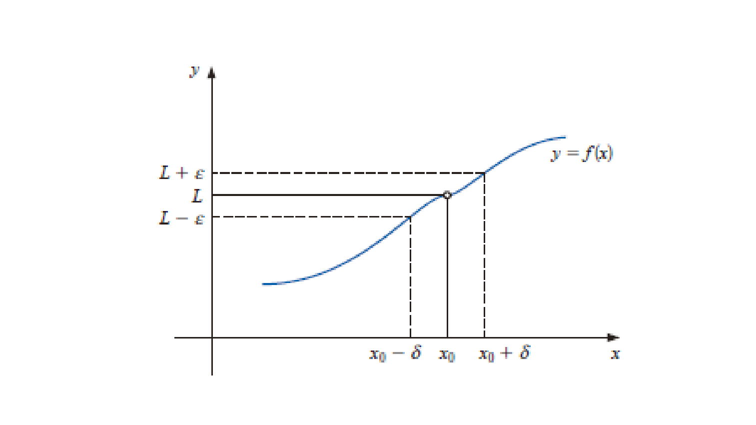

Figure: Fig.1

Definition 1.2

- Let f be a function defined on a set X of real numbers and $x_0 \in X$.
- Then f is **continuous** at x_0 if

$$\lim_{x \to x_0} f(x) = f(x_0).$$

- The function f is continuous on the set X if it is continuous at each number in X.

- Especially, let $C(X)$ denote the set of all functions that are continuous on the set X.
- When X is an closed interval $[a, b]$, the set of all functions that are continuous on the interval $[a, b]$ is denoted by $C[a, b]$.

Definition 1.3

Let $\{x_n\}_{n=1}^{\infty}$ be an infinite sequence of real or complex number. The sequence converges to a number x (Limit) if, for any $\varepsilon > 0$, there exists a positive integer $N(\varepsilon)$, such that implies

$$\left|x_n - x\right| < \varepsilon,$$

whenever $n > N(\varepsilon)$.

Noted by

$$\lim_{n\to\infty} x_n = x,$$

or $x_n \to x$ as $n \to \infty$.

Theorem 1.4

If f is a function defined on a set of real numbers and $x_0 \in X$, then the following statements are equivalent:

a. f is continuous at x_0;

b. if $\{x_n\}_{n=1}^{\infty}$ is any sequence in X converging to x_0, then

$$\lim_{n\to\infty} f(x_n) = f(x_0). \blacksquare$$

Definition 1.5

If f is a function defined in an open interval containing x_0, then f is differentiable at x_0, if

$$f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

exists.

The number $f'(x_0)$ ia called the **derivative** of $f(x)$ at x_0.

Notes:

- $C^n(X)$ denote the set of all functions that have n continuous derivatives on X.
- Especially $C^\infty(X)$ denote the set of all functions that have derivatives of all orders on X

Some Important Theorems

Theorem 1.6

If the function f is differentiable at x_0, then f is continuous at x_0.

Theorem 1.7 (Rolle's Theorem):

- Suppose $f \in C[a, b]$ and f is differentiable on (a, b).
- If $f(a) = f(b) = 0$, then a number c in (a, b) exists with $f'(c) = 0$).

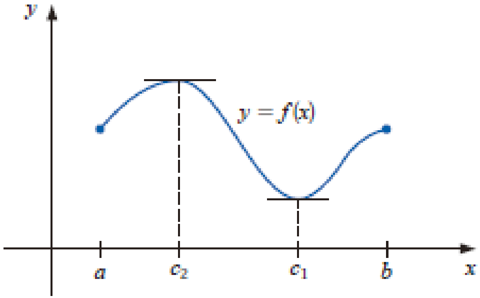

Figure: Fig.2

Theorem 1.8 (Mean Value Theorem – 均值定理)

Suppose $f \in C[a, b]$ and f is differentiable on (a, b),then a number c in (a, b) exists with

$$f'(c) = \frac{f(b) - f(a)}{b - a}.$$

Theorem 1.9 (Extreme Value Theorem – 极值定理)

- If $f \in C[a, b]$, then $c_1, c_2 \in [a, b]$ exist with $f(c_1) \leq f(x) \leq f(c_2)$ for each $x \in [a, b]$.
- If, in addition, f is differentiable on (a, b), then the numbers c_1 and c_2 occur either at the endpoints of $[a, b]$ or where f' is zero.

Definition 1.10

The **Riemann Integral** of a function on an interval $[a, b]$ is the following limit, provided it exists:

$$\int_a^b f(x)\mathrm{d}x = \lim_{\max \Delta x_i \to 0} \sum_{i=1}^{n} f(z_i)\Delta x_i,$$

where the numbers $x_0, x_1, x_2, \cdots, x_n$ satisfy $a = x_0 \leq x_1 \leq x_1 \leq \cdots \leq x_n = b$, and where $\Delta x_i = x_i - x_{i-1}$ for each $i = 1, 2, \cdots, n$ and z_i is an arbitrarily chosen in the interval $[x_{i-1}, x_i]$.

Especially, if we choose $z_i = x_i$ and $\Delta x_i = (b-a)/n$, then in this case

$$\int_a^b f(x)\mathrm{d}x = \lim_{n\to\infty} \frac{b-a}{n} \sum_{i=1}^{n} f(x_i),$$

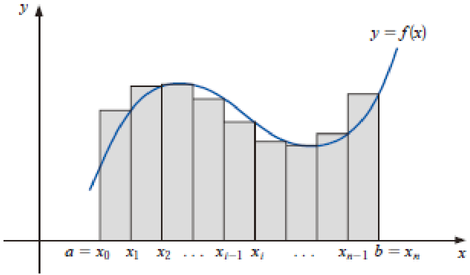

Figure: Fig.3

Theorem 1.11 (Weighted Mean Value Theorem for the Integral)

If $f \in C[a, b]$, the Riemann Integral of g exists on the $[a, b]$, and $g(x)$ does not change sign on $[a, b]$, then there exists a number in (a, b) with

$$\int_a^b f(x)g(x)\mathrm{d}x = f(c)\int_a^b g(x)\mathrm{d}x. \blacksquare$$

When $g(x) \equiv 1$, this theorem give the average value of the function f over the interval $[a, b]$.

$$f(c) = \frac{1}{b-a}\int_a^b f(x)\mathrm{d}x.$$

Theorem 1.12 (Generalized Rolle's Theorem)

Suppose $f \in C[a, b]$ is n times differentiable on (a, b). If $f(x)$ is zero at the $n + 1$ distinct numbers $x_0, x_1, x_2, \cdots, x_n$ in the $[a, b]$, then a number c in the (a, b) exists with

$$f^{(n)}(c) = 0. \blacksquare$$

Theorem 1.13 (Intermediate Value Theorem):

If $f \in C[a, b]$ and K is any number between $f(a)$ and $f(b)$, then there exists a number c in (a, b) for which $f(c) = K$.

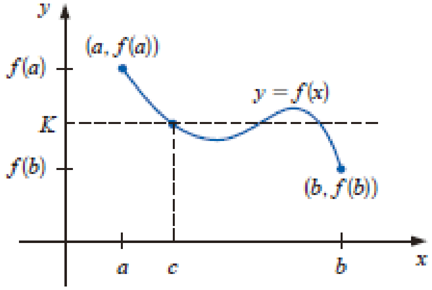

Figure: Fig.4

Theorem 1.14 (Taylor's Theorem)

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

$$\begin{aligned} P_n(x) &= f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 \\ &+ \cdots + \frac{f^n(x_0)}{n!}(x - x_0)^n \\ &= \sum_0^n \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k, \end{aligned}$$

and

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

Example 1: see $(\sqrt{3})^2 = 3$

- this is true in traditional arithmetic in algebra or calculus, but if we use calculator or computer to do, what will happen?
- In our traditional mathematical world, we permit number with an infinite number of digits;
- But in arithmetic, we define $\sqrt{3}$ as an unique positive number, so when it is multiplied by itself, we can get 3.
- In computer computation, $\sqrt{3}$ first is represented with a fixed, finite number of digits, which may be very closed to its exact value. This means only rational (有理数) number can be presented exactly.

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Roundoff error(舍入误差):

- For computer storage, one standard is made by IEEE , which is Binary Floating Arithmetic Standard 754-1985:
- **Format:** single, double, or extended precision
- **64-bit(binary digit) representation for a real number:**
  - **Representation(浮点数格式):**
    由三部分组成：符号+指数+尾数
  - The first bit is a **sign** indicator, denoted s, This is followed by an 11-bit exponent(指数), c, called the **characteristic**, and a 52-bit binary fraction, f, call the **mantissa**(尾数).The base for the exponent is 2.
  - Using this system, a floating-point number can be shown with the form:

$$(-1)^s 2^{c-1023}(1+f)$$

Example 2: consider the machine number

$0\ 10000000011\ 101110010001\underbrace{00\cdots00}$

- s=0
  $c = 1\cdot2^{10}+0\cdot2^9+\cdots+0\cdot2^2+1\cdot2^1+1\cdot2^0 = 1024+2+1 = 1027$
  $f = 1\cdot\left(\frac{1}{2}\right)^1+1\cdot\left(\frac{1}{2}\right)^3+1\cdot\left(\frac{1}{2}\right)^4+1\cdot\left(\frac{1}{2}\right)^5+1\cdot\left(\frac{1}{2}\right)^8+1\cdot\left(\frac{1}{2}\right)^{12}$
- So the machine number precisely represents the decimal number(十进制数)

$$
\begin{aligned}
& (-1)^s 2^{c-1023}(1+f) \\
= & (-1)^0\cdot 2^{1027-1023} \\
& \times\left(1+\frac{1}{2}+\frac{1}{8}+\frac{1}{16}+\frac{1}{32}+\frac{1}{256}+\frac{1}{4096}\right) \\
= & 27.56640625.
\end{aligned}
$$

- **underflow (下溢):** number less than $2^{-1023} \cdot (1 + 2^{-52})$; cause to zero.
- **overflow (上溢):** number greater than $2^{1024} \cdot (2 - 2^{-52})$, cause to halt.
- **Normalized decimal floating-point form:标准十进制浮点数**

$$\pm 0.d_1 d_2 \cdots d_k \times 10^n,$$

where $1 \leq d_1 \leq 9$,and $0 \leq d_i \leq 9$ for each $i = 1, 2, \cdots, k$.

- Numbers of this form are called k-**digit decimal machine numbers**— k位十进制机器数.
- The left digits $d_{k+1} d_{k+2} \cdots$ can be treated by **chopping(截断) or rounding（舍入）methods**.

Definition 1.15

If p^* is an approximation to p, the **absolute error** is $|p - p^*|$, and the **relative error** is $\frac{|p-p^*|}{|p|}$, provided that $p \neq 0$.

Definition 1.16

The number p^* is said to approximate p to t **significant digit**(有效位数) (or figures) if t is the largest nonnegative integer for which

$$\frac{|p - p^*|}{|p|} < 5 \times 10^{-t}.$$

1.3 Algorithms and Convergence

- **Algorithm:** an algorithm is a procedure that describes, in an unambiguous(明确的) or clear manner, a **finite sequence of steps** to be performed in a specified order.
- **Key techniques for algorithm:** looping and condition-control method;
- **Description:** pseudo-code method.

Example 1: to compute $\sum_{i=1}^{n} x_i = x_1 + x_2 + \cdots + x_n$

Algorithm

INPUT: $N, x_1, x_2, \cdots, x_n$.
OUTPUT: SUM$=\sum_{i=1}^{n} x_i$.
Step1 Set SUM=0
Step2 For $i = 1, 2, \cdots, N$ do
    set SUM=SUM$+x_i$
Step 3 OUTPUT (SUM);
    STOP.

Some important concepts on algorithm:Stability

- **Stable(稳定性):** An algorithm is said to be **stable** imply that small changes in the initial data can produce correspondingly small changes in final results.
- Some algorithm are stable only for certain choices of initial data, this case are called **conditionally stable** （条件稳定）.

Definition 1.17

Suppose that E_0 denotes an initial error and E_n represents the magnitude of an error after n subsequent operations.

- If $E_n \approx CnE_0$, where C is a constant independent of n, then the growth of error is said to be **linear**.
- If $E_n \approx C^n E_0$, for some $C > 1$,then the growth of error is called **exponential**.

Definition 1.18

- Suppose $\{\beta_n\}_{n=1}^{\infty}$ is a sequence known to converge to zero, and $\{\alpha_n\}_{n=1}^{\infty}$ converges to a number α.
- If a positive constant K exists with

$$|\alpha_n - \alpha| \leq K|\beta_n|,$$

for large n

- then we say that $\{\alpha_n\}_{n=1}^{\infty}$ converges to α with the **rate of convergence** $O(\beta_n)$, writing $\alpha_n = \alpha + O(\beta_n)$.

误差的传播

记$\hat{p}, \hat{q}$ 分别为p, q 的近似值，误差分别为$\varepsilon_p, \varepsilon_q$

- 和运算：

$$p + q = (\hat{p} + \varepsilon_p) + (\hat{q} + \varepsilon_q) = (\hat{p} + \hat{q}) + (\varepsilon_p + \varepsilon_q)$$

- 积运算：

$$pq = (\hat{p} + \varepsilon_p)(\hat{q} + \varepsilon_q) = \hat{p}\hat{q} + \hat{p}\varepsilon_q + \hat{q}\varepsilon_p + \varepsilon_p\varepsilon_q$$

- 商运算：

$$\frac{p}{q} - \frac{\hat{p}}{\hat{q}} = \frac{\hat{p} + \varepsilon_p}{\hat{q} + \varepsilon_q} - \frac{\hat{p}}{\hat{q}} = -\frac{\hat{p}\varepsilon_q + \hat{q}\varepsilon_p}{\hat{q}(\hat{q} + \varepsilon_q)}$$

Example 2:

Suppose that for $n \geq 1$,

$$\alpha_n = \frac{n+1}{n^2}, \quad \texttt{and} \quad \hat{\alpha}_n = \frac{n+3}{n^3}.$$

we can see that

$$|\alpha_n - 0| = \frac{n+1}{n^2} \leq \frac{n+n}{n^2} = 2\frac{1}{n}$$

and

$$|\hat{\alpha}_n - 0| = \frac{n+3}{n^3} \leq \frac{n+3n}{n^3} \leq 4\frac{1}{n^2}$$

so

$$\alpha_n = 0 + O(\frac{1}{n}), \quad \texttt{and} \quad \hat{\alpha}_n = 0 + O(\frac{1}{n^2}).$$

Definition 1.19

Suppose that

$$\lim_{h\to 0} G(h) = 0$$

and

$$\lim_{h\to 0} F(h) = L.$$

If a positive constant K exists with

$$|F(h) - L| \leq K|G(h)|,$$

for sufficient small h, then we write

$$F(h) = L + O(G(h)).$$

Example 3:

By Taylor formula for sufficient small h, we have

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

since

$$|(\cos h + \frac{1}{2}h^2) - 1| = |\frac{1}{24}h^4 \cos \xi(h)| \leq \frac{1}{24}h^4,$$

so

$$\cos h + \frac{1}{2}h^2 = 1 + O(h^4)$$

Well-Posed or ill-posed Problem—适定性与不适定性问题

A **mathematical Problem** is said to be **well-posed** if a **solution**

1. exists,
2. is unique,
3. depends continuously on problem data .

Otherwise, problem is **ill-posed.**

Remarks:

- Even if problem is well posed, solution may still be **sensitive** to input data.
- Computational algorithm should not make sensitivity worse.

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General Strategy to solve mathematical problems

- Replace difficult problem by easier one having same or closely related solution:
  - infinite $\to$ finite
  - differential $\to$ algebraic
  - nonlinear $\to$ linear
  - complicated $\to$ simple
  - high - order $\to$ low - order
- Solution obtained may only approximate that of original problem

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Remarks:

1. **Accuracy** of final results reflects all these.
2. The **resulting perturbations** during computation may be **amplified**(放大) by algorithm or the nature of problem.
3. The study of the effects of such approximations on the **accuracy** and **stability** of numerical algorithms is traditionally called **error analysis**.

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Remarks:

1. **Accuracy** of final results reflects all these.
2. The **resulting perturbations** during computation may be **amplified**(放大) by algorithm or the nature of problem.
3. The study of the effects of such approximations on the **accuracy** and **stability** of numerical algorithms is traditionally called **error analysis**.

Example: Approximations

Computing surface area of Earth using formula $A = 4\pi r^2$ involves several **approximations**

- Earth is modeled as sphere, idealizing its true shape;
- Value for radius is based on empirical measurements and previous computations;
- Value for π requires truncating infinite process;
- Values for input data and results of arithmetic operations are rounded in computer.

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Remarks:

1. True value usually unknown, so we **estimate or bound error** rather than compute it exactly
2. **Relative error often taken relative to approximate value**, rather than (unknown) true value.

Assignment: