

Numerical Analysis

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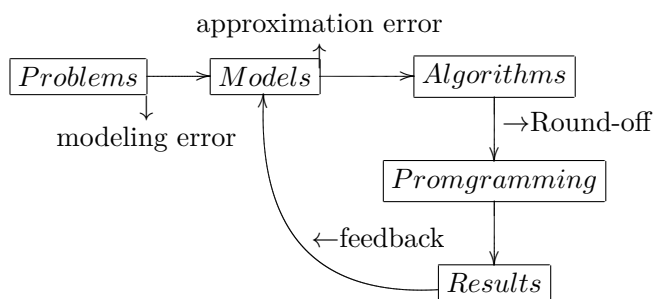
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第零章 Preface

0.1 Preface



第一章 Mathematical Preliminaries and Error Analysis

1.1 Mathematical Preliminaries and Error Analysis

1.1.1 Round-off Errors and Computer Arithmetic

Binary machine numbers

定义 1.1.1 舍入误差 舍入误差形成原因：进行有限位的运算 (*finite digits arithmetic*)

其中，*IEEE:754-2008* 规定二进制机器数 (*Binary machine numbers*) 中浮点数 (*floating-point*) 存储规范如下：

$$(-1)^S 2^{c-1023} (1 + f)$$
$$\begin{cases} S : 0/1 & \text{signpart} \\ c : 11 \text{ digits} & \text{exponential part.} \\ f : 52 \text{ digits} & \text{mantissa part} \end{cases}$$

由于实数的稠密性，可知找不到比某一个数大的最小的数或小的最大的数，但是在计算机中可以找到，所以计算机不能表示所有的数。

Decimal machine numbers

$\pm 0.d_1d_2 \cdots d_n \times 10^n$ 其中 $1 \leq d_1 \leq 9$, $0 \leq d_i \leq 9$, $\forall i \geq 2$ 。如果记真实的数为 y , 其浮点数表示为 $fl(y)$ 。

当存在 $y = 0.d_1d_2 \cdots d_kd_{k+1} \cdots \times 10^n$, 其浮点数表示有如下两种方式:

1. Chopping: chop off digits, say $d_{k+1}d_{k+2} \cdots$.
2. Rounding: $y + 5 \times 10^{n-(k+1)}$, then chopping.

例 1.1.1

$\pi = 3.14159265 \cdots$, 取 5 位。

- Chopping: $fl(y) = 0.31415 \times 10^1$.
- Rounding: $fl(y) = 0.31416 \times 10^1$.

π

定义 1.1.2 Suppose p^* is an approximation of p .

$$\begin{cases} \text{absolute error} &= |p^* - p| \\ \text{relative error} &= \frac{|p^* - p|}{p} \end{cases}$$

定义 1.1.3 有效数字 (Significant digits) p^* is said to approximate p with t significant digits. If t is the largest nonnegative integer, s.t.

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

Chopping floating:

$$y = 0.d_1 \cdots d_k d_{k+1} \cdots \times 10^n$$

$$fl(y) = 0.d_1 \cdots d_k \times 10^n$$

Chopping: (其有效位数至少为 $k-1$)

$$\frac{|fl(y) - y|}{|y|} = \frac{0.0 \cdots 0 d_{k+1} \cdots \times 10^n}{0.d_1 \cdots d_k d_{k+1} \cdots \times 10^n} \leq 10^{1-k}$$

Rounding: (其有效位数至少为 k)

$$\frac{|fl(y) - y|}{|y|} \leq \frac{0.0 \cdots 1 d_{k+1} \cdots \times 10^n}{0.d_1 \cdots d_k d_{k+1} \cdots \times 10^n} \leq 10^{-k}$$

Machine Operators

记计算机的加减乘除为 $\oplus \ominus \otimes \oslash$, 于是有

$$x \oslash y = fl(fl(x) \oslash fl(y))$$

Four cases to avoid:

1. 两个十分接近的数 (two nearly equal)。
2. 分子远大于分母 (numerator » denominator)。
3. 避免大数吃掉小数。

Nested method (秦九韶算法)

```

input :  $a_0, a_1, \dots, a_n(\text{given})$ ;  $x$ 
output:  $P_n(x)$ 

1  $S_n \leftarrow a_n$ ;
2 for  $k \leftarrow n - 2$  to 0 do
3    $S_k \leftarrow x S_{k+1} + a_k$ ;
4 end
5  $P_n(x) \leftarrow S_0$ ;
```

```

1 def nested(poly:list=[1], x:float=0.0)->float:
2     """
3     Horner nested polynomial calculation.
4     """
```


第一章 Mathematical Preliminaries and Error Analysis

```

5      Args:
6          poly: List, store the coefficient of the polynomial.
7          x: Float, specify the variable in the polynomial.
8
9      Returns:
10         Float, result.
11
12     Raises:
13         If 'poly' is empty, raise IndexError.
14         If type(args) does not correspond, raise TypeError.
15     """
16     result = poly[0]
17     for i in range(1, poly.__len__()):
18         result = x*result + poly[i]
19     return result

```

Convergence (收敛性)

Stable: small change in initial data and the error is small.

若 E_0 为初始值误差, E_n 为 n 步的误差,

- $E_n \approx C$ (不依赖 n), 称之为线性。
- $E_n \approx C^n E_0$ 则可由 C 的取值判断是否稳定。

定义 1.1.4 Rates of Convergence 当 $n \rightarrow \infty$, $\alpha_n \rightarrow \alpha$, $\beta_n \rightarrow 0$, 其中 $|\alpha_n - \alpha| \leq k |\beta_n|$ (与 n 的取值无关), 则称 α_n 是以 β_n 的速度收敛到 α 的。

$$\alpha_n = \alpha + o(\beta_n).$$

第二章 Solutions of Equations in One Variable

2.1 Root-finding problem

2.1.1 The Bisection Method

定理 2.1.1 *Intermediate Value Theorem* $f \in [a, b], \forall k \in f([a, b]), \exists c \in [a, b], s.t. f(c) = k$ 。

```
1 def Bisection(fun, a:float, b:float, max_step:int=128, ...
2     eps:float=1e-6)->float:
3     mid_last = a
4     if fun(a)*fun(b) < 0:
5         for i in range(0, max_step):
6             mid = (a+b) / 2
7             if abs(mid-mid_last)<eps or abs(fun(mid))<eps:
8                 print("Step: %d\nZero: %fc"%(i, mid))
9                 return mid
10            else:
11                if fun(mid)*fun(a)<0:
12                    b = mid
13                else:
14                    a = mid
15            mid_last = mid
16    print('Bisection cannot be convergent within..')
```

the pre-set steps.'

定理 2.1.2 $f \in C[a, b]$ (continuous), 根据如上算法, P_i 为 mid 的序列。如果 $\exists \text{ root } P \in [a, b]$, 则有 $|P_n - P| \leq \frac{b-a}{2^n}$ 。

[Proof] $|b_n - a_n| = \frac{b-a}{2^{n-1}}$,

$$|P_n - P| \leq \frac{1}{2}(b_n - a_n) = \frac{b-a}{2^n}$$

于是 $P_n = P + o(2^{-n})$ 。

□

2.1.2 Fixed-Point Iteration

定义 2.1.1 Fixed-point Iteration 对 $g(P)$, 如果 $\forall x \in [a, b]$, 如果 $\exists P$ s.t. $g(P)=P$, 则称 P 为不动点 (fixed point)。

如果 $g(x) \in C[a, b]$ 并且 $g([a, b]) \subset [a, b]$, there exists at least one $p \in [a, b]$, s.t. $g(p)=p$ 。

定理 2.1.3 不动点迭代根的存在唯一性定理 $g(x) \in C[a, b]$, $g([a, b]) \subset [a, b]$ 。 $\forall x \in [a, b]$, 都有 $g'(x) \leq \kappa < 1$ 。

[Proof]

存在性:

$$\begin{cases} h(a) = g(a) - a \geq 0 \\ h(b) = g(b) - b \leq 0 \end{cases}$$

于是有 $h(a)h(b) \leq 0$, 则 $\exists p$, s.t. $h(p)=0$ 。

唯一性:

假设存在两个根 P_1, P_2 , 使得 $P_1 = g(P_1), P_2 = g(P_2)$, 但是 $P_1 \neq P_2$ 。

$$\begin{aligned} |g(P_1) - g(P_2)| &= |g'(\xi)| |P_1 - P_2|, \quad \xi \in [P_1, P_2]. \\ &\leq \kappa |P_1 - P_2|, \text{contradiction.} \end{aligned}$$

□

定理 2.1.4 不动点收敛的充分条件 $g \in C[a, b]$, $g([a, b]) \subset [a, b]$, $g'(x)$ 存在, 并且 $|g'(x)| \leq \kappa < 1$. $\forall P_0 \in [a, b]$, 定义序列 $P_i = g(P_{i-1})$, $i = 1, 2, \dots$, 则 $\lim_{n \rightarrow \infty} P_n = P$ (P 为不动点)。

[Proof]

$$\begin{aligned}
 |P_n - P| &= |g(P_{n-1}) - g(P)| \\
 &= |g'(\xi_{n-1})| |P_{n-1} - P| \\
 &\leq \kappa |P_{n-1} - P| \\
 &\leq \dots \leq \dots \\
 &\leq \kappa^n |P_0 - P| \rightarrow 0.
 \end{aligned}$$

□

其中, 寻找不动点的代码如下:

```

1 def fixed_point(fun, start:float=0, max_step:int=128, ...
2     eps:float=1e-6)->float:
3     new_val = fun(start)
4     for i in range(0, max_step):
5         old_val = new_val
6         new_val = fun(old_val)
7         if -eps < old_val - new_val < eps:
8             print(i)
9             return new_val

```

定理 2.1.5 如果满足定理 2.1.4, 则 p_n 接近 p 的误差可以表示为

$$|P_n - P| \leq \kappa^n \max\{P_0 - a, b - P_0\}$$

并且有

$$\begin{aligned}
 |P_n - P| &= |P_n - P_{n+1} + P_{n+2} - P_{n+3} + \dots| \\
 &\leq |P_n - P_{n+1}| + |P_{n+2} - P_{n+3}| + \dots \\
 &= \kappa^n (1 + \kappa + \kappa^2 + \dots) |P_0 - P_1| \\
 &= \frac{\kappa^n}{1 - \kappa} |P_0 - P_q|
 \end{aligned}$$

2.1.3 Newton's Method and Its Extensions

Suppose that $f \in C^2[a, b]$. $p_0 \in [a, b]$ and $f'(p_0) \neq 0$ and $|p - p_0|$ is small.

$$0 = f(p) = f(p_0) + (p - p_0)f'(p_0) + \frac{(p - p_0)^2}{2}f''(\xi(p)),$$

$|p - p_0|$ is small, the term involving $(p - p_0)^2$ is much smaller, then we will get

$$p \sim p_0 - \frac{f(p_0)}{f'(p_0)} \equiv p_1.$$

This sets the stage for Newton's method. which starts with an initial approximation p_0 and generates the sequence $\{p_n\}_{n=0}^\infty$,

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}, \quad \text{for } n \geq 1.$$

```

1 def Newton_method(f, df, start:float=0.0, max_step:int=32,...
2     sign_dig:int=6)->float:
3     fun = lambda x: x - f(x)/df(x)
4     return fixed_point(fun, start, max_step, sign_dig)
5
6 def fixed_point(fun, start:float, max_step:int,...
7     sign_dig:int)->float:
8     fl = lambda x: round(x, 100)
9     eps = 10**(-sign_dig)
10    new_val = fun(start)
11    for i in range(0, max_step):
12        old_val = fl(new_val)

```

2.1 Root-finding problem

```
13         new_val = fl(fun(old_val))
14         if abs(old_val-new_val)<=2*eps:
15             return (i, new_val)
16     return "Max_step..."
```

定理 2.1.6 牛顿法的收敛性 *Let $f \in C^2[a, b]$. If $p \in (a, b)$ is such that $f(p) = 0$ and $f'(p) \neq 0$, then there exists a $\delta > 0$ such that Newton's method generates a sequence $\{p_n\}_{n=0}^{\infty}$ converging to p for any initial approximation $p_0 \in [p - \delta, p + \delta]$.*

[Proof] 证明基于将牛顿迭代法看作 functional iteration scheme $p_n = g(p_{n-1})$, 既然 $f'(p) \neq 0$, 则 $\exists \delta_1 > 0$ 使得 $f'(x) \neq 0$ 对于所有的 $x \in [p - \delta_1, p + \delta_1]$, 于是有 $g(x) = x - \frac{f(x)}{f'(x)}$ 。求导后有

$$g'(x) = 1 - \frac{f'(x)f'(x) - f(x)f''(x)}{[f'(x)]^2} = \frac{f(x)f''(x)}{[f'(x)]^2}.$$

于是有 $g'(p) = \frac{f(p)f''(p)}{[f'(p)]^2} = 0$, 又因为 g' 是连续的, $0 < k < 1$, 所以 $\exists \delta$, 有 $0 < \delta < \delta_1$, 并且 $|g'(x)| \leq k$, 对于所有的 $x \in [p - \delta, p + \delta]$ 都成立。

接下来需要证明 g 映射 $[p - \delta, p + \delta]$ 到 $[p - \delta, p + \delta]$ 。

$$|g(x) - p| = |g(x) - g(p)| = |g'(\xi)| |x - p| \neq k |x - p| < |x - p| < \delta.$$

综上所述, 存在 $\delta > 0$, 当 $p_0 \in [p - \delta, p + \delta]$ 都有牛顿迭代法收敛到 p 。□

2.1.4 The Secant Method

$$p_n = p_{n-1} - \frac{f(p_{n-1})(p_{n-1} - p_{n-2})}{f(p_{n-1}) - f(p_{n-2})}$$

2.1.5 The Method of False Position

The method generates approximations in the same manner as the Secant method, but it includes a test to ensure that the root is always bracketed between successive iterations.

```

1 def false_position(f, start:list, max_step:int=32, ...
2     eps:float=1e-6) -> float:
3     """
4     False position.
5     -----
6     Args:
7         f: Function.
8         start: List of float, the first iteration point.
9         max_step: Integer, max number of iteration.
10
11     Returns:
12         Float zero.
13         zero / fun(zero)\\sim 0.
14
15     Raises:
16         None.
17     """
18     p = [i for i in start]
19     q = [f(i) for i in start]
20     for i in range(max_step):
21         _p = p[-1] - q[-1]*(p[-1]-p[0])/(q[-1]-q[0])
22         if abs(_p-p[-1]) < eps:
23             return (i, _p)
24         _q = f(_p)
25         if _q*q[-1] < 0:
26             p[0] = p[-1]
27             q[0] = q[-1]
28         p[-1] = _p
29         q[-1] = _q
30     return False

```

2.2 Error Analysis for Iterative Methods

定义 2.2.1 *Order of Convergence* $\{p_n\}_{n=0}^{\infty}$ 是一个收敛到 p 的序列, 但是对于所有的 n 都有 $p_n \neq p$, 如果存在正数 λ, α 满足以下条件:

$$\lim_{n \rightarrow \infty} \frac{|p_{n+1} - p|}{|p_n - p|^\alpha} = \lambda,$$

then $\{p_n\}_{n=0}^{\infty}$ converges to p of order α , with asymptotic error constant λ .

如果 $\alpha = 1$ (and $\lambda < 1$), 则称序列为线性收敛 (*linearly convergent*).

如果 $\alpha = 2$, 则序列为二次收敛 (*quadratically convergent*).

线性收敛: $|p_n - 0| \approx (0.5)^n |p_0|$.

二次收敛: $|\tilde{p}_n - 0| \approx (0.5)^{2^n - 1} |\tilde{p}_0|$.

定理 2.2.1 Let $g \in C[a, b]$ be such that $g(x) \in [a, b]$, for all $x \in [a, b]$. Suppose that g' is continuous on (a, b) and a positive constant $k < 1$ exists with

$$|g'(x)| \leq k, \quad \text{for all } x \in (a, b).$$

If $g'(p) \neq 0$, then for any number $p_0 \neq p$ in $[a, b]$, the sequence

$$p_n = g(p_{n-1}), \quad \text{for } n \geq 1,$$

converges only linearly to the unique fixed point p in $[a, b]$.

[Proof]

$$\begin{aligned} p_{n+1} - p &= g(p_n) - g(p) = g'(\xi_n)(p_n - p), \\ \Rightarrow \lim_{n \rightarrow \infty} \frac{p_{n+1} - p}{p_n - p} &= \lim_{n \rightarrow \infty} g'(\xi_n) = g'(p) \end{aligned}$$

\Rightarrow If $g'(p) \neq 0$, fixed-point iteration exhibits linear convergence with asymptotic error constant $|g'(p)|$. □

定理 2.2.2 *Let p be a solution of the equation $x = g(x)$. Suppose that $g'(p) = 0$ and g'' is continuous with $|g''(x)| < M$ on an open interval I containing p . Then there exists a $\delta > 0$ such that, for $p_0 \in [p - \delta, p + \delta]$, the sequence defined by $p_n = g(p_{n-1})$, when $n \geq 1$, converges at least quadratically to p . Moreover, for sufficiently large values of n ,*

$$|p_{n+1} - p| < \frac{M}{2} |p_n - p|^2.$$

[Proof]

$$g(x) = g(p) + g'(p)(x - p) + \frac{g''(\xi)}{2}(x - p)^2,$$

□

第三章 Interpolation and Polynomial Approximation

3.1 Interpolation and the Lagrange Polynomial

定理 3.1.1 (Weierstrass Approximation Theorem) $f \in C[a, b]$,
 \forall polynomial $P(x)$, s.t. $|f(x) - P(x)| < \epsilon$ for all $x \in [a, b]$.

定理 3.1.2 (nth Lagrange Interpolating Polynomial) x_0, \dots, x_n are $n+1$ distinct numbers, then a unique polynomial $P(x)$ of degree at most n exists with

$$\begin{cases} f(x_k) = P(x_k) \quad \text{for } k = 0 : n \\ P(x) = \sum_{k=0}^n f(x_k) L_{n,k}(x) \\ L_{n,k} = \prod_{\substack{i=0 \\ i \neq k}}^n \frac{(x-x_i)}{x_k-x_i} \\ L_{n,k}(x_j) = \delta_{k,j} \end{cases}$$

If $f \in C^{n+1}[a, b]$, $\exists \xi(x) \in (a, b)$, s.t.

$$f(x) = P(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^n (x-x_i)$$

[Proof] let

$$g(t) = f(t) - P(t) - [f(x) - g(x)] \prod_{i=0}^n \frac{(t - x_i)}{x - x_i},$$

$g(t)$ satisfies

$$\begin{cases} g(x_k) = 0 & k = 0 : n \\ g(x) = 0 \\ g \in C^{n+1}[a, b] \end{cases}$$

By *Generalized Rolle's Theorem*, $\exists \xi \in (a, b)$, s.t. $g^{(n+1)}(\xi) = 0$, then we have

$$\begin{aligned} 0 &= g^{(n+1)}(\xi) = f^{(n+1)}(\xi) - P^{(n+1)}(\xi) - [f(x) - P(x)] \frac{d^{n+1}}{dt^{n+1}} \left[\prod_{i=0}^n \frac{(t - x_i)}{x - x_i} \right]_{t=\xi} \\ \Rightarrow 0 &= f^{(n+1)}(\xi) - [f(x) - P(x)] \frac{(n+1)!}{\prod_{i=0}^n (x - x_i)} \\ \Rightarrow f(x) &= P(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^n (x - x_i). \end{aligned}$$

□

3.2 Data Approximation and Neville's Method

定义 3.2.1 The Lagrange Polynomial that agrees with $f(x)$ at the k distinct points $x_{m_1}, x_{m_2}, \dots, x_{m_k}$ is denoted $P_{m_1, m_2, \dots, m_k}(x)$.

定理 3.2.1 Let f be defined at x_0, x_1, \dots, x_k , then

$$P(x) = \frac{(x - x_j)P_{0, \dots, j-1, j+1, \dots, k}(x) - (x - x_i)P_{0, \dots, i-1, i+1, \dots, k}(x)}{x_i - x_j}$$

is the k th Lagrange polynomial that interpolates f at the $k+1$ points.

3.2.1 Neville's Method

To avoid the multiple subscripts, we let $Q_{i,j}$ ($0 \leq j \leq i$) denote the interpolating polynomial of degree j on the $(j+1)$ numbers x_{i-j}, \dots, x_i .

$$Q_{i,j} = P_{i-j, i-j+1, \dots, i-1, i}$$

then for $i = 1 : n$, $j = 1 : i$,

$$Q_{i,j} = \frac{(x - x_{i-j})Q_{i,j-1} - (x - x_i)Q_{i-1,j-1}}{x_i - x_{i-j}}$$

3.3 Divided Differences

3.3.1 Divided Differences Notation

The k th divided difference relative to x_i, \dots, x_{i+k} is

$$\begin{aligned} f[x_i] &= f(x_i) \\ f[x_i, \dots, x_{i+k}] &= \frac{f[x_{i+1}, \dots, x_{i+k}] - f[x_i, \dots, x_{i+k-1}]}{x_{i+k} - x_i} \end{aligned}$$

for each $k = 0, 1, \dots, n$, $P_n(x)$ can be rewritten in a form called *Newton's Divided-Difference*:

$$P_n(x) = f[x_0] + \sum_{k=1}^n f[x_0, \dots, x_k](x - x_0) \cdots (x - x_{k-1})$$

定理 3.3.1 $f \in C^n[a, b]$, $x_i \in [a, b]$ for $i = 0 : n$, $\exists \xi \in (a, b)$, s.t.

$$f[x_0, x_1, \dots, x_n] = \frac{f^{(n)}(\xi)}{n!}$$

[Proof] Let $g(x) = f(x) - P_n(x)$, which has $n+1$ distinct zeros in $[a, b]$. According to *Generalized Rolle's Theorem*, $\exists \xi \in (a, b)$, s.t. $g^{(n)}(\xi) = 0$.

$$\begin{aligned} 0 &= g^{(n)}(\xi) = f^{(n)}(\xi) - P_n^{(n)}(\xi) = f^{(n)}(\xi) - n!f[x_0, \dots, x_n] \\ \Rightarrow f[x_0, x_1, \dots, x_n] &= \frac{f^{(n)}(\xi)}{n!} \end{aligned}$$

□

When the nodes are arranged consecutively with equal spacing, then we use $h = x_{i+1} - x_i$ and $x = s \cdot h + x_0$, the equation will become

$$\begin{aligned} P_n(x) &= P_n(x_0 + sh) = f[x_0] + \sum_{k=1}^n s(s-1)\cdots(s-k+1)h^k f[x_0, \dots, x_k] \\ &= f[x_0] + \sum_{k=1}^n \binom{s}{k} k! h^k f[x_0, \dots, x_k]. \end{aligned}$$

3.3.2 Forward Differences

$$\begin{aligned} f[x_0, x_1] &= \frac{1}{h} (f(x_1) - f(x_0)) = \frac{1}{h} \Delta f(x_0) \\ f[x_0, x_1, x_2] &= \frac{1}{2h} \left(\frac{\Delta f(x_1) - \Delta f(x_0)}{h} \right) = \frac{1}{2h^2} \Delta^2 f(x_0) \end{aligned}$$

In general,

$$\begin{aligned} f[x_0, x_1, \dots, x_k] &= \frac{1}{k! h^k} \Delta^k f(x_0) \\ \Rightarrow P_n(x) &= f[x_0] + \sum_{k=1}^n \binom{s}{k} \Delta^k f(x_0) \end{aligned}$$

3.3.3 Backward Differences

$$\begin{aligned} f[x_n, x_{n-1}] &= \frac{1}{h} \nabla f(x_n) \\ f[x_n, x_{n-1}, x_{n-2}] &= \frac{1}{2h^2} \nabla^2 f(x_n) \end{aligned}$$

In general,

$$\begin{aligned} f[x_n, x_{n-1}, \dots, x_{n-k}] &= \frac{1}{k! h^k} \nabla^k f(x_n) \\ \Rightarrow P_n(x) &= f[x_n] + \sum_{k=1}^n \frac{s(s+1)\cdots(s+k-1)}{k!} \nabla^k f(x_n) \end{aligned}$$

Also, we have

$$\binom{-s}{k} = \frac{-s(-s-1)\cdots(-s-k+1)}{k!} = (-1)^k \frac{s(s+1)\cdots(s+k-1)}{k!}$$

$$\Rightarrow P_n(x) = f[x_n] + \sum_{k=1}^n (-1)^k \binom{-s}{k} \nabla^k f(x_n)$$

3.3.4 Centered Differences

$$\begin{aligned} P_n(x) = P_{2m+1}(x) &= f[x_0] + \frac{sh}{2} (f[x_{-1}, x_0] + f[x_0, x_1]) + (sh)^2 f[x_{-1}, x_0, x_1] \\ &+ \cdots \\ &+ s^2(s^2-1)\cdots(s^2-(m-1)^2)h^{2m}f[x_{-m}, \cdots, x_{m+1}] \\ &+ \frac{s^2(s^2-1)\cdots(s^2-m^2)h^{2m+1}}{2} (f[x_{-m-1}, \cdots, x_m] + f[x_{-m}, \cdots, x_{m+1}]) \end{aligned}$$

If $n = 2m + 1$ is odd, we use the above formula, if $n = 2m$ is even, we delete the last line and then use the above formula.

x	f(x)	1st	2nd	3rd	4th divided differences
x_{-2}	$f[x_{-2}]$	$f[x_{-2}, x_{-1}]$	$f[x_{-2}, x_{-1}, x_0]$	$f[x_{-2}, x_{-1}, x_0, x_1]$	$f[x_{-2}, x_{-1}, x_0, x_1, x_2]$
x_{-1}	$f[x_{-1}]$	$f[x_{-1}, x_0]$	$f[x_{-1}, x_0, x_1]$	$f[x_{-1}, x_0, x_1, x_2]$	
x_0	$f[x_0]$	$f[x_0, x_1]$	$f[x_0, x_1, x_2]$		
x_1	$f[x_1]$	$f[x_1, x_2]$			
x_2	$f[x_2]$				

3.4 Hermite Interpolation

The osculating polynomial approximating a function $f \in C^m[a, b]$ at x_i for each $i = 0 : n$, of which the derivatives of order less than or equal to m_i , then the degree of this osculating polynomial is at most $M = \sum_{i=0}^n m_i + n$.

$$\frac{d^k P(x_i)}{dx^k} = \frac{d^k f(x_i)}{dx^k}, \quad \text{for each } i = 0 : n, k = 0 : m_i.$$

$$\begin{cases} n = 0 & m_0 \text{ Taylor polynomial for } f \text{ at } x_0 \\ m_i = 0 (\text{each } i) & \text{nth Lagrange polynomial} \end{cases}$$

3.4.1 Hermite Polynomials

定理 3.4.1 $f \in C'[a, b]$ and $x_0, \dots, x_n \in [a, b]$, the unique polynomial of least degree agreeing with f and f' at x_0, \dots, x_n is the Hermite polynomial of degree at most $2n + 1$.

$$H_{2n+1}(x) = \sum_{j=0}^n f(x_j) H_{n,j}(x) + \sum_{j=0}^n f'(x_j) \hat{H}_{n,j}(x)$$

$$\begin{cases} H_{n,j}(x) &= [1 - 2(x - x_j)L'_{n,j}(x_j)] L_{n,j}^2(x) \\ \hat{H}_{n,j}(x) &= (x - x_j)L_{n,j}^2(x) \end{cases}$$

Moreover, if $f \in C^{2n+2}[a, b]$, then

$$f(x) = H_{2n+1}(x) + \frac{(x - x_0)^2 \cdots (x - x_n)^2}{(2n + 2)!} f^{(2n+2)}(\xi(x)).$$

[Proof]

$$\begin{aligned} H_{n,j}(x_i) &= \delta_{i,j} & \hat{H}_{n,j}(x_i) &= 0 \\ H'_{n,j}(x_i) &= 0 & \hat{H}'_{n,j}(x_i) &= \delta_{i,j} \end{aligned}$$

□

3.4.2 Hermite Polynomials Using Divided Differences

Suppose that the distinct numbers x_0, \dots, x_n are given together with values of f and f' . Define a new sequence z_0, \dots, z_{2n+1} by

$$z_{2i} = z_{2i+1} = x_i \quad \text{for } i = 0 : n.$$

We have $H_{2n+1}(x) = f[z_0] + \sum_{k=1}^{2n+1} f[z_0, \dots, z_k](x - z_0) \cdots (x - z_{k-1})$.

z	$f(z)$	First divided differences	\cdots
$z_0 = x_0$	$f[z_0] = f(x_0)$	$f[z_0, z_1] = f'(x_0)$	\vdots
$z_1 = x_0$	$f[z_1] = f(x_0)$	$f[z_1, z_2] = \frac{f[z_2] - f[z_1]}{z_2 - z_1}$	\vdots
$z_2 = x_1$	$f[z_2] = f(x_1)$	$f[z_2, z_3] = f'(x_1)$	\vdots
$z_3 = x_1$	$f[z_3] = f(x_1)$	$f[z_3, z_4] = \frac{f[z_4] - f[z_3]}{z_4 - z_3}$	\vdots
$z_4 = x_2$	$f[z_4] = f(x_2)$	$f[z_4, z_5] = f'(x_2)$	
$z_5 = x_2$	$f[z_5] = f(x_2)$		

3.5 Cubic Spline Interpolation

定义 3.5.1 Given a function f defined on $[a, b]$, $a = x_0 < x_1 < \cdots < x_n = b$, a cubic spline interpolation S for f is a function that satisfies the following conditions.

1. $S_j(x)$ is a cubic polynomial, on the subinterval $[x_j, x_{j+1}]$ for $j = 0 : n - 1$.
2. $S_j(x_j) = f(x_j)$, $S_j(x_{j+1}) = f(x_{j+1})$ for $j = 0 : n - 2$.
3. $S'_j(x_{j+1}) = S'_{j+1}(x_{j+1})$ for $j = 0 : n - 2$.
4. $S''_j(x_{j+1}) = S''_{j+1}(x_{j+1})$ for $j = 0 : n - 2$.
5. $\begin{cases} \text{natural boundary:} & S''(x_0) = S''(x_n) = 0. \\ \text{clamped boundary:} & S'(x_0) = f'(x_0), S'(x_n) = f'(x_n). \end{cases}$

3.5.1 Construction of a Cubic Spline

Let $h_j = x_{j+1} - x_j$ (forward):

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(1)

$$\begin{aligned} S_j(x) &= a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3 \quad \text{for } j = 0 : n - 1 \\ \Rightarrow a_{j+1} &= S_{j+1}(x_{j+1}) = S_j(x_{j+1}) \\ &= a_j + b_j h_j + c_j h_j^2 + d_j h_j^3 = f(x_{j+1}) \quad \text{for } j = 0 : n - 1 \end{aligned}$$

(2)

$$\begin{aligned} S'_j(x) &= b_j + 2c_j(x - x_j) + 3d_j(x - x_j)^2 \\ \Rightarrow b_{j+1} &= S'_{j+1}(x_{j+1}) = S'_j(x_{j+1}) \\ &= b_j + 2c_j h_j + 3d_j h_j^2 \quad \text{for } j = 0 : n - 1 \end{aligned}$$

(3)

$$\begin{aligned} S''_j(x) &= 2c_j + 6d_j(x - x_j) \\ \Rightarrow 2c_{j+1} &= S''_{j+1}(x_{j+1}) = S''_j(x_{j+1}) \\ &= 2c_j + 6d_j h_j \quad \text{for } j = 0 : n - 1 \end{aligned}$$

Above all, the linear system to be solved is:

$$Ax = b$$

$$\begin{cases} A = \text{diag}([1, 2(h_0 + h_1), \dots, 2(h_{n-2} + h_{n-1}), 1]) \\ \quad + \text{diag}([0, h_1, \dots, h_{n-1}], 1) + \text{diag}([h_0, \dots, h_{n-2}, 0], -1) \\ x = [c_0; c_1; \dots; c_n] \\ b = \left[0; \frac{3}{h_1}(a_2 - a_1) - \frac{3}{h_0}(a_1 - a_0); \dots; \frac{3}{h_{n-1}}(a_n - a_{n-1}) - \frac{3}{h_{n-2}}(a_{n-1} - a_{n-2}); 0\right] \end{cases}$$

Then we will get b_j, d_j by

$$\begin{cases} b_j &= \frac{1}{h_j}(a_{j+1} - a_j) - \frac{h_j}{3}(2c_j + c_{j+1}) \\ d_j &= \frac{1}{3h_j}(c_{j+1} - c_j) \end{cases}$$

3.5 Cubic Spline Interpolation

3.5.2 Clamped Splines

$$Ax = b$$

$$\left\{ \begin{array}{l} A = \begin{pmatrix} 2h_0 & h_0 & 0 & \cdots & 0 \\ h_0 & 2(h_0 + h_1) & h_1 & \ddots & \vdots \\ 0 & h_1 & 2(h_1 + h_2) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & h_{n-1} \\ 0 & \cdots & \cdots & h_{n-1} & 2h_{n-1} \end{pmatrix} \\ x = (c_0 \quad c_1 \quad \cdots \quad c_n)^T \\ b = \begin{pmatrix} \frac{3}{h_0}(a_1 - a_0) - 3f'(a) \\ \frac{3}{h_1}(a_2 - a_1) - \frac{3}{h_0}(a_1 - a_0) \\ \vdots \\ \frac{3}{h_{n-1}}(a_n - a_{n-1}) - \frac{3}{h_{n-2}}(a_{n-1} - a_{n-2}) \\ 3f'(b) - \frac{3}{h_{n-1}}(a_n - a_{n-1}) \end{pmatrix} \end{array} \right.$$

第四章 Numerical Differentiation and Integration

4.1 Numerical Differentiation

To approximate $f'(x)$ ($x_0 \in (a, b)$, $f \in C^2[a, b]$), $x_1 = x_0 + h \in [a, b]$.

$$\begin{aligned}
 f(x) &= P_{0,1}(x) + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x)) \\
 &= \frac{f(x_0)(x-x_0-h)}{-h} + \frac{f(x_0)(x-x_0)}{h} + \frac{(x-x_0)(x-x_1)}{2} f''(\xi(x)) \\
 \Rightarrow f'(x) &= \frac{f(x_0+h) - f(x_0)}{h} + \frac{2(x-x_0)-h}{2} f''(\xi(x)) + \frac{(x-x_0)(x-x_0-h)}{2} D_x(f''(\xi(x))) \\
 \Rightarrow f'(x_0) &= \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2} f''(\xi)
 \end{aligned}$$

The above formula is known as the forward-difference formula if $h > 0$, and the backward-difference formula if $h < 0$.

定理 4.1.1 ((n+1)-point Formula) $\{x_0, x_1, \dots, x_n\}$ are $(n+1)$ dis-

inct numbers in interval I , $f \in C^{n+1}(I)$.

$$\begin{aligned}
 f(x) &= \sum_{k=0}^n f(x_k) L_k(x) + \prod_{k=0}^n \left(\frac{x - x_k}{k+1} \right) f^{(n+1)}(\xi(x)). \\
 \Rightarrow f'(x) &= \sum_{k=0}^n f(x_k) L'_k(x) + D_x \left[\prod_{k=0}^n \left(\frac{x - x_k}{k+1} \right) \right] f^{(n+1)}(\xi(x)) \\
 &\quad + \prod_{k=0}^n \left(\frac{x - x_k}{k+1} \right) D_x [f^{(n+1)}(\xi(x))]. \\
 \Rightarrow f'(x_j) &= \sum_{k=0}^n f(x_k) L'_k(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{\substack{k=0 \\ k \neq j}}^n (x_j - x_k).
 \end{aligned}$$

4.1.1 Three-Point Formulas

If the nodes are equally spaced, $x_1 = x_0 + h$, $x_2 = x_0 + 2h$, then

- Three-Point Formula

$$f'(x_0) = \frac{1}{h} \left[\frac{1}{2} f(x_0) - 2f(x_0 + h) + \frac{3}{2} f(x_0 + 2h) \right] + \frac{h^2}{3} f^{(3)}(\xi_0).$$

- Three-Point Endpoint Formula

$$f'(x_0) = \frac{1}{h} \left[-\frac{3}{2} f(x_0) + 2f(x_0 + h) - \frac{1}{2} f(x_0 + 2h) \right] + \frac{h^2}{3} f^{(3)}(\xi_1).$$

- Three-Point Midpoint Formula

$$f'(x_0) = \frac{1}{h} \left[-\frac{1}{2} f(x_0) + \frac{1}{2} f(x_0 + 2h) \right] - \frac{h^2}{6} f^{(3)}(\xi_2).$$

4.1.2 Five-Point Formulas

- Five-Point Midpoint Formula

$$\begin{aligned}
 f'(x_0) &= \frac{1}{12h} [f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) \\
 &\quad - f(x_0 + 2h)] + \frac{h^4}{30} f^{(5)}(\xi).
 \end{aligned}$$

- Five-Point Endpoint Formula

$$\begin{aligned}
 f'(x_0) &= \frac{1}{12h} [-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) \\
 &\quad + 16f(x_0 + 3h) - 3f(x_0 + 4h)] + \frac{h^4}{5} f^{(5)}(\xi).
 \end{aligned}$$

4.1.3 Second Derivative Midpoint Formula

$$f''(x_0) = \frac{1}{h} [f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12} f^{(4)}(\xi)$$

If $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$, it is also bounded, and the approximation is $O(h^2)$.

4.1.4 Round-Off Error Instability

$$f'(x_0) = \frac{1}{2h} [f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6} f^{(3)}(\xi_1)$$

Suppose that in evaluating $f(x_0 + h)$ and $f(x_0 - h)$ we encounter round-off errors $e(x_0 + h)$ and $e(x_0 - h)$.

$$f(x_0 + h) = \tilde{f}(x_0 + h) + e(x_0 + h) \quad \text{and} \quad f(x_0 - h) = \tilde{f}(x_0 - h) + e(x_0 - h)$$

The total error in the approximation

$$\begin{aligned} \left| f'(x_0) - \frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} \right| &= \left| \frac{e(x_0 + h) - e(x_0 - h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1) \right| \\ &\leq \frac{\varepsilon}{h} + \frac{h^2}{6} M, \end{aligned}$$

where $e(x_0 \pm h)$ are bounded by $\varepsilon > 0$ and $f^{(3)}$ are bounded by $M > 0$. There is an optimal h such that the bound is small.

4.2 Richardson's Extrapolation

Suppose that for each number $h \neq 0$, we have a formula $N_1(h)$ that approximates an unknown constant M with truncation error $O(h)$

$$\begin{aligned} M - N_1(h) &= K_1 h + K_2 h^2 + K_3 h^3 + \dots \\ M - N_1\left(\frac{h}{2}\right) &= K_1 \frac{h}{2} + K_2 \frac{h^2}{4} + K_3 \frac{h^3}{8} + \dots \end{aligned}$$

If we subtract the first equation from the second equation, then we'll get

$$\begin{aligned}
 M &= N_1 \left(\frac{h}{2} \right) + \left[N_1 \left(\frac{h}{2} - N_1(h) \right) \right] + K_2 \left(\frac{h^2}{2} - h^2 \right) + K_3 \left(\frac{h^3}{4} - h^3 \right) + \dots \\
 \Rightarrow N_2(h) &= N_1 \left(\frac{h}{2} \right) + \left[N_1 \left(\frac{h}{2} - N_1(h) \right) \right] \\
 \Rightarrow M &= N_2(h) - \frac{K_2}{2} h^2 - \frac{3K_3}{4} h^3 + \dots \quad \text{with truncation error } O(h^2)
 \end{aligned}$$

$$\begin{aligned}
 M &= N_2 \left(\frac{h}{2} \right) + \left[N_2 \left(\frac{h}{2} - N_2(h) \right) \right] / 3 + \frac{K_3}{8} h^3 + \dots \\
 \Rightarrow N_3(h) &= N_2 \left(\frac{h}{2} \right) + \left[N_2 \left(\frac{h}{2} - N_2(h) \right) \right] / 3 \\
 \Rightarrow M &= N_3(h) - \frac{K_3}{8} h^3 + \frac{7K_3}{48} h^4 + \dots \quad \text{with truncation error } O(h^3)
 \end{aligned}$$

4.3 Elements of Numerical Integration

$$\begin{aligned}
 \int_a^b f(x) dx &= \int_a^b \sum_{i=0}^n f(x_i) L_i(x) dx + \int_a^b \prod_{i=0}^n (x - x_i) \frac{f^{(n+1)}(\xi(x))}{(n+1)!} dx \\
 &= \int_a^b a_i f(x_i) dx + \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^n (x - x_i) f^{(n+1)}(\xi(x)) dx,
 \end{aligned}$$

where $a_i = \int_a^b L_i(x) dx$ for each $i = 0, 1, \dots, n$.

4.3.1 The Trapezoidal Rule

To derive the Trapezoidal rule for approximating $\int_a^b f(x) dx$, let $x_0 = a$, $x_1 = b$, $h = b - a$.

$$\begin{aligned}
 \int_a^b f(x) dx &= \int_a^b \left[\frac{(x - x_0)}{(x_1 - x_0)f(x_1)} + \frac{(x - x_1)}{(x_0 - x_1)f(x_0)} \right] dx + \frac{1}{2} \int_a^b (x - x_0)(x - x_1) f''(\xi(x)) dx \\
 &= \int_{x_0}^{x_1} \frac{(x - x_0)f(x_1) - (x - x_1)f(x_0)}{x_1 - x_0} dx + \frac{f''(\xi)}{2} \left[\frac{x^3}{3} - \frac{(x_0 + x_1)}{2} x^2 + x_0 x_1 x \right]_{x_0}^{x_1} \\
 &= \left[\frac{(x - x_0)^2 f(x_1) - (x - x_1)^2 f(x_0)}{2(x_0 - x_1)} \right]_{x_0}^{x_1} - \frac{h^3}{12} f''(\xi) \\
 &= \frac{h}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi).
 \end{aligned}$$

4.3.2 Simpson's Rule

$$\begin{aligned}
 \int_{x_0}^{x_2} f(x)dx &= \left[f(x_1)(x - x_1) + \frac{f'(x_1)}{2}(x - x_1)^2 + \frac{f''(x_1)}{6}(x - x_1)^3 + \frac{f^{(3)}(x_1)}{24}(x - x_1)^4 \right]_{x_0}^{x_2} \\
 &\quad + \frac{1}{24} \int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4 dx \\
 &= 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \frac{f^{(4)}(\xi_1)}{60}h^5 \\
 &= 2hf(x_1) + \frac{h^3}{3} \left\{ \frac{1}{h^2} [f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12}f^{(4)}(\xi_2) \right\} + \frac{f^{(4)}(\xi_1)}{60}h^5 \\
 &= \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{12} \left[\frac{1}{3}f^{(4)}(\xi_2) - \frac{1}{5}f^{(4)}(\xi_1) \right] \\
 &= \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90}f^{(4)}(\xi)
 \end{aligned}$$

4.3.3 Measuring Precision

定义 4.3.1 (The degree of accuracy or precision)

The largest positive integer n such that the formula is exact for x^k for $k = 0, 1, \dots, n$.

4.3.4 Newton-Cotes Formulas

The Trapezoidal and Simpson's rules are examples of a class of methods known as Newton-Cotes formulas. There are two types of Newton-Cotes formulas, open and closed.

Closed Newton-Cotes Formulas

The $(n + 1)$ -point closed Newton-Cotes uses nodes $x_i = x_0 + ih$, for $i = 0, 1, \dots, n$, where $x_0 = a$, $x_n = b$ and $h = (b - a)/n$.

定理 4.3.1 *If n is even and $f \in C^{n+2}[a, b]$*

$$\int_a^b f(x)dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1) \dots (t-n) dt.$$

If n is odd and $f \in C^{n+1}[a, b]$

$$\int_a^b f(x)dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1) \dots (t-n) dt.$$

$$\xi \in (a, b).$$

n=1 Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi)$$

n=2 Simpson's rule

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi)$$

n=3 Simpson's Three-Eighths rule

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8} [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80} f^{(4)}(\xi)$$

n=4

$$\int_{x_0}^{x_4} f(x)dx = \frac{2h}{45} [7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)] - \frac{8h^7}{945} f^{(6)}(\xi)$$

Open Newton-Cotes Formulas

The open Newton-Cotes formulas do not include the endpoints of $[a, b]$ as nodes. They use the nodes $x_i = x_0 + ih$, for $i = 0, 1, \dots, n$, where $h = (b - a)/(n + 2)$ and $x_0 = a + h$, $x_n = b - h$.

定理 4.3.2 *If n is even and $f \in C^{n+2}[a, b]$*

$$\int_a^b f(x)dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2(t-1)\dots(t-n)dt.$$

If n is odd and $f \in C^{n+1}[a, b]$

$$\int_a^b f(x)dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_{-1}^{n+1} t(t-1)\dots(t-n)dt.$$

$$\xi \in (a, b).$$

n=0 Midpoint rule

$$\int_{x_{-1}}^{x_1} f(x)dx = 2hf(x_0) + \frac{h^3}{3} f''(\xi)$$

n=1

$$\int_{x_{-1}}^{x_2} f(x)dx = \frac{3h}{2} [f(x_0) + f(x_1)] - \frac{3h^3}{4} f''(\xi)$$

n=2

$$\int_{x_{-1}}^{x_3} f(x)dx = \frac{4h}{3} [2f(x_0) - f(x_1) + 2f(x_2)] + \frac{14h^5}{45} f^{(4)}(\xi)$$

n=3

$$\int_{x_{-1}}^{x_4} f(x)dx = \frac{5h}{24} [11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)] + \frac{95h^7}{144} f^{(4)}(\xi)$$

4.4 Composite Numerical Integration

To calculate an arbitrary integral $\int_a^b f(x)dx$, choose an even integer n , subdivide the interval $[a, b]$ into n subinterval, and apply Simpson's rule on

each consecutive pair of subintervals. With $h = (b - a)/h$ and $x_j = a + jh$, for $j = 0, 1, \dots, n$, we have

$$\begin{aligned}
 \int_a^b f(x)dx &= \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)dx \\
 &= \sum_{j=1}^{n/2} \left\{ \frac{h}{3} [f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})] - \frac{h^5}{90} f^{(4)}(\xi_j) \right\} \\
 &= \frac{h}{3} \left[f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right] - \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \\
 &= \frac{h}{3} [\dots\dots] - \frac{h^5}{90} \left(\frac{n}{2} \right) f^{(4)}(\mu) \\
 &= \frac{h}{3} [\dots\dots] - \frac{(b-a)}{180} h^4 f^{(4)}(\mu)
 \end{aligned}$$

定理 4.4.1 (Composite Simpson's Rule) Let $f \in C^4[a, b]$, n be even, $h = \frac{b-a}{n}$, and $x_j = a + jh$ for $j = 0, 1, \dots, n$. There exists a $\mu \in (a, b)$ s.t. with n subintervals

$$\begin{aligned}
 \int_a^b f(x)dx &= \frac{h}{3} \left[f(a) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + f(b) \right] \\
 &\quad - \frac{b-a}{180} h^4 f^{(4)}(\mu).
 \end{aligned}$$

定理 4.4.2 (Composite Trapezoidal Rule) Let $f \in C^2[a, b]$, n be even, $h = \frac{b-a}{n}$, and $x_j = a + jh$ for $j = 0, 1, \dots, n$. There exists a $\mu \in (a, b)$ s.t. with n subintervals

$$\int_a^b f(x)dx = \frac{h}{2} \left[f(a) + 2 \sum_{j=1}^{n-1} f(x_j) + f(b) \right] - \frac{b-a}{12} h^2 f''(\mu).$$

定理 4.4.3 (Composite Midpoint Rule) Let $f \in C^2[a, b]$, n be even, $h = \frac{b-a}{n+2}$, and $x_j = a + (j+1)h$ for $j = -1, 0, \dots, n+1$. There exists a $\mu \in (a, b)$ s.t. with $n+2$ subintervals

$$\int_a^b f(x)dx = 2h \sum_{j=0}^{n/2} f(x_{2j}) + \frac{b-a}{6} h^2 f''(\mu).$$

4.4.1 Round-off Error Stability

$$\begin{aligned} e(h) &= \left| \frac{h}{3} \left[e_0 + 2 \sum_{j=1}^{n/2-1} e_{2j} + 4 \sum_{j=1}^{n/2} e_{2j-1} + e_n \right] \right| \\ &\leq \frac{h}{3} \left[|e_0| + 2 \sum_{j=1}^{n/2-1} |e_{2j}| + 4 \sum_{j=1}^{n/2} |e_{2j-1}| + |e_n| \right] \\ &\leq \frac{h}{3} \left[\varepsilon + 2\left(\frac{n}{2} - 1\right)\varepsilon + 4\left(\frac{n}{2}\right)\varepsilon + \varepsilon \right] = \frac{h}{3} 3h\varepsilon = nh\varepsilon \\ &= (b-a)\varepsilon. \end{aligned}$$

If the round-off errors are uniformly bounded by ε .

4.5 Romberg Integration

Romberg

To approximate the integral $I = \int_a^b f(x) dx$, select an integer $n > 0$.

INPUT endpoints a, b ; integer n .

OUTPUT an array R . (Compute R by rows; only the last 2 rows are saved in storage.)

Step 1 Set $h = b - a$;
 $R_{1,1} = \frac{h}{2}(f(a) + f(b)).$

Step 2 OUTPUT $(R_{1,1})$.

Step 3 For $i = 2, \dots, n$ do Steps 4–8.

4.6 Gaussian Quadrature

$$\textbf{Step 4} \quad \text{Set } R_{2,1} = \frac{1}{2} \left[R_{1,1} + h \sum_{k=1}^{2^{i-2}} f(a + (k - 0.5)h) \right].$$

(Approximation from Trapezoidal method.)

Step 5 For $j = 2, \dots, i$

$$\text{set } R_{2,j} = R_{2,j-1} + \frac{R_{2,j-1} - R_{1,j-1}}{4^{j-1} - 1}. \quad (\text{Extrapolation.})$$

Step 6 OUTPUT ($R_{2,j}$ for $j = 1, 2, \dots, i$).

Step 7 Set $h = h/2$.

Step 8 For $j = 1, 2, \dots, i$ set $R_{1,j} = R_{2,j}$. (Update row 1 of R .)

Step 9 STOP.

4.6 Gaussian Quadrature

4.6.1 Legendre Polynomial

定理 4.6.1 Suppose x_1, x_2, \dots, x_n are the roots of the n th Legendre polynomial $P_n(x)$ and that for $i = 1, 2, \dots, n$ the number C_i are defined by

$$C_i = \int_{-1}^1 \prod_{\substack{j=1 \\ j \neq i}}^n \left(\frac{x - x_j}{x_i - x_j} \right) dx.$$

If $P(x)$ is any polynomial of degree less than $2n$, then

$$\int_{-1}^1 P(x) dx = \sum_{i=1}^n C_i P(x_i)$$

[Proof]

(1) $P(x)$ is of degree less than n .

$$\begin{aligned} \int_{-1}^1 P(x) dx &= \int_{-1}^1 \sum_{i=1}^n P(x_i) L_i(x) dx = \int_{-1}^1 \sum_{i=1}^n \prod_{\substack{j=1 \\ j \neq i}}^n \left(\frac{x - x_j}{x_i - x_j} \right) P(x_i) dx \\ &= \sum_{i=1}^n \left[\int_{-1}^1 \prod_{\substack{j=1 \\ j \neq i}}^n \left(\frac{x - x_j}{x_i - x_j} \right) dx \right] P(x_i) = \sum_{i=1}^n C_i P(x_i). \end{aligned}$$

(2) $P(x)$ is of degree at least n but less than $2n$.

$$P(x_i) = Q(x_i)P_n(x_i) + R(x_i) = R(x_i) \quad (\text{degree less than } n).$$

□

4.6.2 Gaussian Quadrature on Arbitrary Intervals

An integral $\int_a^b f(x)dx$ over an arbitrary $[a, b]$ can be transformed into an integral over $[-1, 1]$

$$\int_a^b f(x)dx = \int_{-1}^1 f\left(\frac{(b-a)t + (b+a)}{2}\right) \frac{(b-a)}{2} dt.$$

第五章 Initial-Value Problems for Ordinary Differential Equations

5.1 The Elementary Theory of Initial-Value Problems

定义 5.1.1 (Lipschitz Condition) *A function $f(t, y)$ is said to satisfy a Lipschitz condition in the variable Y on a set $D \subset \mathbb{R}^2$ if a constant $L > 0$ exists with*

$$|f(t, y_1) - f(t, y_2)| \leq L |y_1 - y_2|$$

whenever $(t_1, y_1), (t_2, y_2)$ are in D . The constant L is called a Lipschitz constant for f .

定义 5.1.2 (Convex) *A set $D \subset \mathbb{R}^2$ is said to be convex if whenever $(t_1, y_1), (t_2, y_2) \in D$, then for every $\lambda \in [0, 1]$,*

$$((1 - \lambda)t_1 + \lambda t_2, (1 - \lambda)y_1 + \lambda y_2) \in D.$$

定理 5.1.1 *Suppose $f(t, y)$ is defined on a convex set $D \subset \mathbb{R}^2$, if a*

constant $L > 0$ exists with

$$\left| \frac{\partial f}{\partial y}(t, y) \right| \leq L$$

for all $(t, y) \in D$, then f satisfies a Lipschitz condition on D in the variable y with Lipschitz constant L .

定理 5.1.2 Suppose that $D = \{(t, y) | a \leq t \leq b, y \in \mathbb{R}\}$ and $f(t, y)$ is continuous on D . If f satisfies a Lipschitz condition on D in the variable y , then the initial-value problem

$$\begin{cases} y'(t) = f(t, y) & a \leq t \leq b \\ y(a) = \alpha \end{cases}$$

has a unique solution $y(t)$ for $a \leq t \leq b$.

5.1.1 Well-Posed Problems

定理 5.1.3 (Well-Posed) Suppose that $D = \{(t, y) | a \leq t \leq b, y \in \mathbb{R}\}$ and $f(t, y)$, if f is continuous and satisfies a Lipschitz condition in the variable y on the set D , then the initial-value problem

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha$$

is well-posed.

5.2 Euler's Method

The object of *Euler's method* is to obtain approximations to the well-posed initial-value problem

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha$$

We will use Taylor's Theorem to derive Euler's method. Suppose that $y(t)$, the unique solution has two continuous derivations on $[a, b]$, so that for each

5.2 Euler's Method

$$i = 0, 1, \dots, N - 1$$

$$y(t_{i+1}) = y(t_i) + (t_{i+1} - t_i)y'(t_i) + \frac{(t_{i+1} - t_i)^2}{2}y''(\xi_i)$$

for some number ξ_i in t_i, t_{i+1} . Because $h = t_{i+1} - t_i$, we have

$$y(t_{i+1}) = y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(\xi_i)$$

Euler's method constructs $\omega_i \approx y(t_i)$, for each $i = 1, 2, \dots, N$, by deleting the remainder term, then Euler's method is

$$\begin{cases} \omega_0 = \alpha \\ \omega_{i+1} = \omega_i + hf(t_i, \omega_i) \quad \text{for } i = 0, 1, \dots, N - 1 \end{cases}$$

5.2.1 Errors Bounds for Euler's Method

定理 5.2.1 Suppose f is continuous and satisfies a Lipschitz condition with constant L on

$$D = \{(t, y) | a \leq t \leq b, y \in \mathbb{R}\}$$

and that a constant M exists with

$$|y''(t)| \leq M, \quad \text{for all } t \in [a, b]$$

where $y(t)$ denotes the unique solution to the initial-value problem

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha$$

Let $\omega_0, \dots, \omega_N$ be the approximations generated by Euler's method for some positive integer N , then for each $i = 0, 1, \dots, N$

$$|y(t_i) - \omega_i| \leq \frac{hM}{2L} [e^{L(t_i-a)} - 1].$$

[Proof]

$$\begin{aligned}
 |y_{i+1} - \omega_{i+1}| &\leq |y_i - \omega_i| + h |f(t_i, y_i) - f(t_i, \omega_i)| + \frac{h^2}{2} |y''(\xi_i)| \\
 &\leq (1 + hL) |y_i - \omega_i| + \frac{h^2 M}{2} \\
 &\leq e^{(i+1)hL} (|y_0 - \omega_0| + \frac{h^2 M}{2hL}) - \frac{h^2 M}{2hL} \\
 &= \frac{hM}{2L} (e^{(t_{i+1}-a)L} - 1).
 \end{aligned}$$

□

定理 5.2.2 *If u_0, u_1, \dots, u_N be the approximations and $|\delta_i| < \delta$, then*

$$|y(t_i) - u_i| \leq \frac{1}{L} \left(\frac{hM}{2} + \frac{\delta}{h} \right) [e^{L(t_i-a)} - 1] + \delta e^{L(t_i-a)}$$

The minimal value of $E(f)$ occurs when $h = \sqrt{\frac{2\delta}{M}}$

5.3 Higher-Order Taylor Method

定义 5.3.1 (Local Truncation Error) *The difference method*

$$\begin{cases} \omega_0 = \alpha \\ \omega_{i+1} = \omega_i + h\phi(t_i, \omega_i) \end{cases} \quad \text{for each } i = 0, 1, \dots, N-1$$

has local truncation error

$$\tau_{i+1}(x) = \frac{y_{i+1} - (y_i + h\phi(t_i, y_i))}{h} = \frac{y_{i+1} - y_i}{h} - \phi(t_i, y_i)$$

for each $i = 0, 1, \dots, N-1$ where y_i and y_{i+1} denote the accuracy at a specific step, assuming that the method was exact at the previous step.

Euler's method has $\tau_{i+1} = \frac{h}{2} y''(\xi_i)$, so the local truncation error in Euler's method is $O(h)$.

5.3.1 Taylor Method of Order n

$$\begin{cases} \omega_0 = \alpha \\ \omega_{i+1} = \omega_i + h\phi(t_i, \omega_i) \quad \text{for each } i = 0, 1, \dots, N-1 \end{cases}$$

where $T^{(n)}(t_i, \omega_i) = f(t_i, \omega_i) + \frac{h}{2}f'(t_i, \omega_i) + \dots + \frac{h^{n-1}}{n!}f^{(n-1)}(t_i, \omega_i)$.

定理 5.3.1 *If Taylor's method of order n is used to approximate the solution to*

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha$$

with step size h and if $y \in C^{n+1}[a, b]$, then the local truncation error is $O(h^n)$.

[Proof]

$$\begin{aligned} y_{i+1} &= y_i + hf(t_i, y_i) + \dots + \frac{h^n}{n!}f^{(n-1)}(t_i, y_i) + \frac{h^{n+1}}{(n+1)!}f^{(n)}(\xi_i, y(\xi_i)) \\ \Rightarrow \tau_{i+1}(h) &= \frac{y_{i+1} - y_i}{h} - T^{(n)}(t_i, y_i) = \frac{h^n}{(n+1)!}f^{(n)}(\xi_i, y(\xi_i)) \end{aligned}$$

for each $i = 0, 1, \dots, N-1$. Since $y \in C^{n+1}[a, b]$, we have $y^{(n+1)}(t) = f^{(n)}(t, y(t))$ bounded on $[a, b]$ and $\tau_i(h) = O(h^n)$ for each $i = 1, 2, \dots, N$.

□

5.4 Runge-Kutta Methods

定理 5.4.1 *Suppose that $f(t, y)$ and all its partial derivatives of order less or equal to $n+1$ are continuous on $D = \{(t, y) | a \leq t \leq b, c \leq y \leq d\}$ ($D = [a, b] \times [c, d]$) and let $(t_0, y_0) \in D$. For every $(t, y) \in D$, there exists ξ between t and t_0 and μ between y and y_0 with*

$$f(t, y) = P_n(t, y) + R_n(t, y)$$

where

$$\begin{aligned}
 P_n(t, y) = & f(t_0, y_0) + \left[(t - t_0) \frac{\partial f}{\partial t}(t_0, y_0) + (y - y_0) \frac{\partial f}{\partial y}(t_0, y_0) \right] \\
 & + \left[\frac{(t - t_0)^2}{2} \frac{\partial^2 f}{\partial t^2}(t_0, y_0) + (t - t_0)(y - y_0) \frac{\partial^2 f}{\partial t \partial y}(t_0, y_0) + \frac{(y - y_0)^2}{2} \frac{\partial^2 f}{\partial y^2}(t_0, y_0) \right] \\
 & + \left[\frac{1}{n!} \sum_{j=0}^{n+1} \binom{n}{j} (t - t_0)^{n-j} (y - y_0)^j \frac{\partial^{n+1} f}{\partial t^{n+1} \partial y^j}(t_0, y_0) \right]
 \end{aligned}$$

$$\text{and } R_n(t, y) = \frac{1}{(n+1)!} \sum_{j=0}^{n+1} \binom{n+1}{j} (t - t_0)^{n+1-j} (y - y_0)^j \frac{\partial^{n+1} f}{\partial t^{n+1} \partial y^j}(\xi, \mu)$$

The function $P_n(t, y)$ is called the n th Taylor polynomial in two variables for the function f about (t_0, y_0) , and $R_n(t, y)$ is the remainder term associated with $P_n(t, y)$.

5.4.1 Runge-Kutta Methods of Order Two

$$\begin{cases} y_{n+1} = y_n + h(c_1 k_1 + c_2 k_2) \\ k_1 = f(x_n, y_n) \\ k_2 = f(x_n + \lambda_2 h, y_n + \mu_{21} h k_1) \end{cases}$$

$$\begin{aligned}
 T_{n+1} &= y(x_{n+1}) - y(x_n) - h[c_1 f(x_n, y_n) + c_2 f(x_n + \lambda_2 h, y_n + \mu_{21} h f_n)] \\
 &= h f_n + \frac{h^2}{2} [f'_x(x_n, y_n) + f'_y(x_n, y_n) f_n] \\
 &\quad - h [c_1 f_n + c_2 (f_n + \lambda_2 f'_x(x_n, y_n) h + \mu_{21} f'_y(x_n, y_n) f_n h)] + O(h^3) \\
 &= (1 - c_1 - c_2) f_n h + \left(\frac{1}{2} - c_2 \lambda_2 \right) f'_x(x_n, y_n) h^2 \\
 &\quad + \left(\frac{1}{2} - c_2 \mu_{21} \right) f'_y(x_n, y_n) f_n h^2 + O(h^3) \\
 &\Rightarrow y_{n+1} = y_n + h f \left(x_n + \frac{h}{2}, y_n + \frac{h}{2} f(x_n, y_n) \right)
 \end{aligned}$$

5.4 Runge-Kutta Methods

5.4.2 Midpoint Method

$$\begin{cases} \omega_0 = \alpha \\ \omega_{i+1} = \omega_i + hf\left(t_i + \frac{h}{2}, \omega_i + \frac{h}{2}f(t_i, \omega_i)\right) \end{cases} \quad \text{for } i = 0, \dots, N-1$$

Local truncation error: $O(h^2)$.

5.4.3 Modified Euler Method

$$\begin{cases} \omega_0 = \alpha \\ \omega_{i+1} = \omega_i + \frac{h}{2} [f(t_i, \omega_i), f(t_{i+1}, \omega_i + hf(t_i, \omega_i))] \end{cases} \quad \text{for } i = 0, \dots, N-1$$

5.4.4 Higher-Order Runge-Kutta Methods

Runge-Kutta Order Three:

$$\begin{cases} \omega_0 = \alpha \\ k_1 = hf(t_i, \omega_i) \\ k_2 = hf\left(t_i + \frac{h}{2}, \omega_i + \frac{1}{2}k_1\right) \\ k_3 = hf(t_i + h, \omega_i - k_1 + 2k_2) \\ \omega_{i+1} = \omega_i + \frac{1}{6}(k_1 + 4k_2 + k_3) \end{cases}$$

Runge-Kutta Order Four:

$$\begin{cases} \omega_0 = \alpha \\ k_1 = hf(t_i, \omega_i) \\ k_2 = hf\left(t_i + \frac{h}{2}, \omega_i + \frac{1}{2}k_1\right) \\ k_3 = hf\left(t_i + \frac{h}{2}, \omega_i - k_1 + \frac{1}{2}k_2\right) \\ k_4 = hf(t_i + h, \omega_i + k_3) \\ \omega_{i+1} = \omega_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \end{cases}$$

5.4.5 Computational Comparisons

Evaluations per step	$n \in [2, 4]$	$n \in [5, 7]$	$n \in [8, 9]$	$n \in [10, \infty]$
Best possible local truncation error	$O(h^n)$	$O(h^{n-1})$	$O(h^{n-2})$	$O(h^3)$

5.5 Error Control and the Runge-Kutta-Fehlberg Method

5.5.1 收敛性与相容性

定义 5.5.1 (收敛) 若一种数值方法, 对于固定的 $x_n = x_0 + nh$, 当 $h \rightarrow 0$ 时有 $y_n \rightarrow y(x_n)$, 其中 $y(x)$ 是初值问题的精确解, 则称该方法是收敛的

定理 5.5.1 (整体截断误差) 假设单步法具有 p 阶精度, 且增量函数 $\varphi(x, y, h)$ 关于 y 满足 Lipschitz 条件

$$|\varphi(x, y, h) - \varphi(x, \bar{y}, h)| \leq L_\varphi |y - \bar{y}|.$$

又设初值 y_0 是准确的, 即 $y_0 = y(x_0)$, 则其整体截断误差

$$y(x_n) - y_n = O(h^p).$$

[Proof] 设以 \bar{y}_{n+1} 表示取 $y_n = y(x_n)$ 用公式求得的结果, 即

$$\bar{y}_{n+1} = y(x_n) + h\varphi(x_n, y(x_n), h),$$

则局部截断误差满足, 存在常数 C , 使 (p 阶精度)

$$|y(x_{n+1}) - \bar{y}_{n+1}| \leq Ch^{p+1}$$

所以有

$$\begin{aligned} |\bar{y}_{n+1} - y_{n+1}| &\leq |y(x_n) - y_n| + h |\varphi(x_n, y(x_n), h) - \varphi(x_n, y_n, h)| \\ &\leq (1 + hL_\varphi) |y(x_n) - y_n|, \end{aligned}$$

5.5 Error Control and the Runge-Kutta-Fehlberg Method

从而有

$$\begin{aligned} |y(x_{n+1}) - y_{n+1}| &\leq |\bar{y}_{n+1} - y_{n+1}| + |y(x_{n+1}) - \bar{y}_{n+1}| \\ &\leq (1 + hL_\varphi) |y(x_n) - y_n| + Ch^{p+1} \end{aligned}$$

即对整体截断误差 $e_n = y(x_n) - y_n$ 成立下列递推关系

$$\begin{aligned} |e_n| &\leq (1 + hL_\varphi) |e_{n-1}| + Ch^{p+1} \\ &\leq (1 + hL_\varphi)^n |e_0| + \frac{Ch^p}{L_\varphi} [(1 + hL_\varphi)^n - 1] \end{aligned}$$

再注意到当 $x_n - x_0 = nh \leq T$ 时,

$$(1 + hL_\varphi)^n \leq (e^{hL_\varphi})^n \leq e^{TL_\varphi}$$

最终有

$$|e_n| \leq |e_0| e^{TL_\varphi} + \frac{Ch^p}{L_\varphi} (e^{TL_\varphi} - 1)$$

由此可以断定, 如果初值准确, 即 $e_0 = 0$, 证毕。 \square

定义 5.5.2 相容 若单步法的增量函数 φ 满足 $\varphi(x, y, 0) = f(x, y)$, 则称单步法与初值问题是相容的。

定义 5.5.3 稳定 若一种数值方法在节点值 y_n 上大小为 δ 的扰动, 于以后各节点值 $y_m (m > n)$ 上产生的偏差不超过 δ , 则称该方法是稳定的。

为了只考虑数值方法本身, 通常只检验将数值方法用于解模型方程的稳定性, 模型方程为

$$y' = \lambda y.$$

其中 λ 为复数, 这个方程分析简单, 对一般方程可以通过局部线性优化转化为这种形式, 例如在 \bar{x}, \bar{y} 的邻域, 可展开为

$$y' = f(x, y) = f(\bar{x}, \bar{y}) + f'_x(\bar{x}, \bar{y})(x - \bar{x}) + f'_y(\bar{x}, \bar{y})(y - \bar{y}) + \cdots$$

定义 5.5.4 单步法对于解模型方程, 若得到的解 $y_{n+1} = E(h\lambda)y_n$, 满足 $|E(h\lambda)| < 1$, 则称该单步法是绝对稳定的, 在 $\mu = h\lambda$ 的平面上, 使 $|E(h\lambda)| < 1$ 的变量围成的区域, 称为绝对稳定域, 它与实轴的交称为绝对稳定区间。

欧拉法	$E(h\lambda) = 1 + h\lambda$
二阶 R-K 方法	$E(h\lambda) = 1 + h\lambda + \frac{(h\lambda)^2}{2}$
三阶 R-K 方法	$E(h\lambda) = 1 + h\lambda + \frac{(h\lambda)^2}{2} + \frac{(h\lambda)^3}{6}$
四阶 R-K 方法	$E(h\lambda) = 1 + h\lambda + \frac{(h\lambda)^2}{2} + \frac{(h\lambda)^3}{6} + \frac{(h\lambda)^4}{24}$
后退欧拉法	$E(h\lambda) = \frac{1}{1-h\lambda}$
梯形法	$E(h\lambda) = \frac{2+h\lambda}{2-h\lambda}$

5.6 Multistep Method

定义 5.6.1 An m -step multistep method for solving the initial-value problem

$$y' = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha$$

] has a difference equation for finding the approximation ω_{i+1} at the mesh point t_{i+1} represented by the following equation, where m is an integer greater than 1:

$$\begin{aligned} \omega_{i+1} = & a_{m-1}\omega_i + a_{m-2}\omega_{i-1} + \cdots + a_0\omega_{i+1-m} \\ & + h[b_m f(t_{i+1}, \omega_{i+1}) + b_{m-1}f(t_i, \omega_i) \\ & + \cdots + b_0 f(t_{i+1-m}, \omega_{i+1-m})] \end{aligned}$$

for $i = m-1, m, \cdots, N-1$, where $h = \frac{b-a}{N}$, the $a_0, a_1, \cdots, a_{m-1}$ and b_0, b_1, \cdots, b_m are constant, and the starting values

$$\omega_0 = \alpha_0, \quad \omega_1 = \alpha_1, \cdots, \omega_{m-1} = \alpha_{m-1}$$

are specified.

$\left\{ \begin{array}{l} \text{When } b_m = 0, \text{ the method is called explicit, or open.} \\ \text{When } b_m \neq 0, \text{ the method is called implicit, or closed.} \end{array} \right.$

第六章 Direct Methods for Solving Linear Systems

6.1 Linear Systems of Equations and Pivoting Strategies

6.1.1 Gaussian Elimination with Backward Substitution

$$\begin{aligned} E1 : & a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = a_{1,n+1} \\ E2 : & a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = a_{2,n+1} \\ & \vdots \\ En : & a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = a_{n,n+1} \end{aligned}$$

6.1.2 Operation Counts

Multiplications / divisions

$$\sum_{i=1}^{n-1} (n-i) + (n-i)(n-i+1) = \frac{2n^3 + 3n^2 - 5n}{6}$$

6.1 Linear Systems of Equations and Pivoting Strategies

Additions / subtractions

$$\sum_{i=1}^{n-1} (n-i)(n-i+1) = \frac{n^3 - n}{3}$$

6.1.3 Backward substitution *&/

$$1 + \sum_{i=1}^{n-1} ((n-i) + 1) = \frac{n^2 + n}{2}$$

6.1.4 Backward substitution +&-

$$\sum_{i=1}^{n-1} ((n-i-1) + 1) = \frac{n^2 - n}{2}$$

6.1.5 Gaussian Elimination with Partial Pivoting

```
1 def gaussian_elimination_partial_pivoting(A, b):
2     np_result = A**-1 * b
3     print(np_result.T)
4     n = A.shape[0]
5     x = np.zeros((n,1))
6     tmp = 0
7     for k in range(n-1):
8         M = k
9         for m in range(k+1,n):
10             if A[m,k] > A[M,k]: M = m
11         A[[k,M]] = A[[M,k]]
12         b[[k,M]] = b[[M,k]]
13         for i in range(k+1,n):
14             m = A[i,k] / A[k,k]
15             for j in range(k,n):
16                 A[i,j] = A[i,j] - m*A[k,j]
17             b[i,0] = b[i,0] - m*b[k,0]
```

```

18     x[-1,0] = b[-1,0] / A[-1,-1]
19     for i in range(n-2,-1,-1):
20         for j in range(i+1,n):
21             tmp += A[i,j] * x[j,0]
22             x[i,0] = (b[i,0] - tmp) / A[i,i]
23             tmp = 0
24     return x

```

6.1.6 Gaussian Elimination with Scaled Partial Pivoting

```

1 def gaussian_elimination_scaled_partial_pivoting(A, b):
2     np_result = A**-1 * b
3     print(np_result.T)
4     n = A.shape[0]
5     x = np.zeros((n,1))
6     tmp = 0
7     for k in range(n):
8         M = np.max(A[k,:])
9         A[k,:] /= M
10        b[k,0] /= M
11    for k in range(n-1):
12        for i in range(k+1,n):
13            m = A[i,k] / A[k,k]
14            for j in range(k,n):
15                A[i,j] = A[i,j] - m*A[k,j]
16                b[i,0] = b[i,0] - m*b[k,0]
17    x[-1,0] = b[-1,0] / A[-1,-1]
18    for i in range(n-2,-1,-1):
19        for j in range(i+1,n):
20            tmp += A[i,j] * x[j,0]
21            x[i,0] = (b[i,0] - tmp) / A[i,i]
22            tmp = 0
23    return x

```

6.2 Matrix Factorization

定理 6.2.1 *If Gaussian elimination can be performed on the linear system $Ax = b$ without row interchanges, then the matrix A can be factored into the product of a lower-triangular matrix L and an upper-triangular matrix U , that is $A = LU$, where $m_{ji} = a_{ji}^{(i)} / a_{ii}^{(i)}$*

$$L = \begin{pmatrix} a_{11}^{(1)} & a_{12}^{(1)} & \cdots & a_{1n}^{(1)} \\ 0 & a_{22}^{(2)} & \ddots & \vdots \\ \vdots & \ddots & \ddots & a_{n-1,n}^{(n-1)} \\ 0 & \cdots & 0 & a_{nn}^{(n)} \end{pmatrix} \quad U = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ m_{21} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ m_{n1} & \cdots & m_{n,n-1} & 1 \end{pmatrix}$$

第七章 Iterative Techniques in Matrix Algebra

7.1 Norms of Vectors and Matrices

定义 7.1.1 A vector norm on \mathbb{R}^n is a function, $\|\cdot\|$, from \mathbb{R}^n to \mathbb{R} with the following properties.

- (i) $\|\mathbf{x}\| \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$.
- (ii) $\|\mathbf{x}\| = 0$ if and only if $\mathbf{x} = \mathbf{0}$.
- (iii) $\|\alpha\mathbf{x}\| = |\alpha| \|\mathbf{x}\|$ for all $\alpha \in \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^n$.
- (iv) $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$ for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$.

定义 7.1.2 The l_1 , l_2 , l_∞ norms for the vector $\mathbf{x} = (x_1, x_2, \dots, x_n)^t$ are defined by

- $\|\mathbf{x}\|_1 = \sum_{i=1}^n |x_i|$
- $\|\mathbf{x}\|_2 = [\sum_{i=1}^n x_i^2]^{1/2}$
- $\|\mathbf{x}\|_\infty = \max_{1 \leq i \leq n} |x_i|$

定理 7.1.1 The sequence of vectors $\mathbf{x}^{(k)}$ converges to \mathbf{x} in \mathbb{R}^n with respect to the l_∞ norm if and only if $\lim_{k \rightarrow +\infty} x_i^{(k)} = x_i$, for each

$$i = 1, 2, \dots, n.$$

7.1.1 Matrix Norms and Distances

定义 7.1.3 (Matrix Norms) A matrix norm on the set of all $n \times n$ matrices is a real-valued function, $\|\cdot\|$, defined on this set, satisfying for all $n \times n$ matrices \mathbf{A} and \mathbf{B} and all real numbers α .

$$(i) \quad \|\mathbf{A}\| \geq 0.$$

$$(ii) \quad \|\mathbf{A}\| = 0 \text{ if and only if } \mathbf{A} \text{ is } \mathbf{0}, \text{ the matrix with all 0 entries.}$$

$$(iii) \quad \|\alpha\mathbf{A}\| = |\alpha| \|\mathbf{A}\|.$$

$$(iv) \quad \|\mathbf{A} + \mathbf{B}\| \leq \|\mathbf{A}\| + \|\mathbf{B}\|.$$

$$(v) \quad \|\mathbf{AB}\| \leq \|\mathbf{A}\| \|\mathbf{B}\|.$$

定理 7.1.2 If $\|\cdot\|$ is a vector norm on \mathbb{R} , then

$$\|\mathbf{A}\| = \max_{\|\mathbf{x}\|=1} \|\mathbf{Ax}\|$$

is a matrix norm.

定理 7.1.3 If $\mathbf{A} = (a_{ij})$ is an $n \times n$ matrix, then

$$\|\mathbf{A}\|_{\infty} = \max_{1 \leq i \leq n} \sum_{j=1}^n |a_{ij}|.$$

7.2 Eigenvalues and Eigenvectors

If \mathbf{A} is a square matrix, the *characteristic polynomial* of \mathbf{A} is defined by $p(\lambda) = \det(\mathbf{A} - \lambda\mathbf{I})$, the zeros of p are *eigenvalues*, or characteristic values, of the matrix \mathbf{A} .

7.2.1 Spectral Radius

定义 7.2.1 (Spectral Radius) The spectral radius $\rho(\mathbf{A})$ of a matrix \mathbf{A} is defined by

$$\rho(\mathbf{A}) = \max |\lambda|, \quad \text{where } \lambda \text{ is an eigen value of } \mathbf{A}.$$

(For complex $\lambda = \alpha + \beta i$, we define $|\lambda| = (\alpha^2 + \beta^2)^{1/2}$.)

定理 7.2.1 If \mathbf{A} is an $n \times n$ matrix, then

- (i) $\|\mathbf{A}\|_1 = \max_j \sum_{i=1}^n |a_{ij}|$, (列和最大)
- (ii) $\|\mathbf{A}\|_2 = [\rho(\mathbf{A}^t \mathbf{A})]^{1/2}$,
- (iii) $\|\mathbf{A}\|_\infty = \max_i \sum_{j=1}^n |a_{ij}|$, (行和最大)
- (iv) $\rho(\mathbf{A}) \leq \|\mathbf{A}\|$, for any natural norm $\|\cdot\|$.

7.2.2 Convergent Matrices

定义 7.2.2 (Convergent) We call an $n \times n$ matrix \mathbf{A} convergent if

$$\lim_{k \rightarrow \infty} (\mathbf{A}^k)_{ij} = 0, \quad \text{for each } i = 1, 2, \dots, n \text{ and } j = 1, 2, \dots, n.$$

定理 7.2.2 The following statements are equivalent

- (i) \mathbf{A} is a convergent matrix.
- (ii) $\lim_{n \rightarrow \infty} \|\mathbf{A}^n\| = 0$, for some natural norm.
- (iii) $\lim_{n \rightarrow \infty} \|\mathbf{A}^n\| = 0$, for all natural norms.
- (iv) $\rho(\mathbf{A}) < 1$.
- (v) $\lim_{n \rightarrow \infty} \mathbf{A}^n \mathbf{x} = \mathbf{0}$, for every \mathbf{x} .

7.3 The Jacobi and Gauss-Siedel Iterative Techniques

7.3.1 Jacobi's Method

The *Jacobi iterative method* is obtained by solving the i th equation in $\mathbf{Ax} = \mathbf{b}$ for x_i to obtain (provided $a_{ii} \neq 0$)

$$x_i = \sum_{\substack{j=1 \\ j \neq i}}^n \left(-\frac{a_{ij}x_j}{a_{ii}} \right) + \frac{b_i}{a_{ii}}, \quad \text{for } i = 1, 2, \dots, n.$$

In general, iterative techniques for solving linear systems by converting the system $\mathbf{Ax} = \mathbf{b}$ into an equivalent system of the form $\mathbf{x} = \mathbf{Tc}$ for some fixed matrix \mathbf{T} and vector \mathbf{c} . After the initial vector $\mathbf{x}^{(0)}$ is selected, the sequence of approximate solution vectors is generated by computing

$$\mathbf{x}^{(k)} = \mathbf{T}\mathbf{x}^{(k-1)} + \mathbf{c}.$$

For Jacobi method, $\mathbf{A} = \mathbf{D}(\mathbf{iag}) - \mathbf{L}(\mathbf{ower}) - \mathbf{U}(\mathbf{pper})$. Then

$$\mathbf{x} = \mathbf{D}^{-1}(\mathbf{L} + \mathbf{U})\mathbf{x} + \mathbf{D}^{-1}\mathbf{b}$$

7.3.2 The Gauss-Seidel Method

$$x_i^{(k)} = \frac{1}{a_{ii}} \left[-\sum_{j=1}^{i-1} (a_{ij}x_j^{(k)}) - \sum_{j=i+1}^n (a_{ij}x_j^{(k-1)}) + b_i \right]$$

That is

$$(\mathbf{D} - \mathbf{L})\mathbf{x}^{(k)} = \mathbf{U}\mathbf{x}^{(k-1)} + \mathbf{b}$$

Then

$$\mathbf{x}^{(k)} = (\mathbf{D} - \mathbf{L})^{-1}\mathbf{U}\mathbf{x}^{(k-1)} + (\mathbf{D} - \mathbf{L})^{-1}\mathbf{b}$$

7.3.3 General Iterative Methods

To study the convergence of general iteration techniques, we need to analyze the formula.

$$\mathbf{x}^{(k)} = \mathbf{T}\mathbf{x}^{(k-1)} + \mathbf{c}$$

引理 7.3.1 *If the spectral radius satisfies $\rho(\mathbf{T}) < 1$, then $(\mathbf{I} - \mathbf{T})^{-1}$ exists, and*

$$(\mathbf{I} - \mathbf{T})^{-1} = \mathbf{I} + \mathbf{T} + \mathbf{T}^2 + \dots = \sum_{j=0}^{\infty} \mathbf{T}^j.$$

定理 7.3.1 *For any $x^{(0)} \in \mathbb{R}^n$, the sequence $\{x^{(k)}\}_{k=0}^{\infty}$ defined by*

$$\mathbf{x}^{(k)} = \mathbf{T}\mathbf{x}^{(k-1)} + \mathbf{c}, \quad \text{for each } k \geq 1$$

converges to the unique solution of $\mathbf{x} = \mathbf{T}\mathbf{x} + \mathbf{c}$ if and only if $\rho(\mathbf{T}) < 1$.

推论 7.3.1 *If $\|\mathbf{T}\| < 1$ for any natural matrix*

(i)

$$\|\mathbf{x} - \mathbf{x}^{(k)}\| \leq \|\mathbf{T}\|^k \|\mathbf{x}^{(0)} - \mathbf{x}\|$$

(ii)

$$\|\mathbf{x} - \mathbf{x}^{(k)}\| \leq \frac{\|\mathbf{T}\|^k}{1 - \|\mathbf{T}\|} \|\mathbf{x}^{(1)} - \mathbf{x}^{(0)}\|$$

定理 7.3.2 (Stein-Rosenberg) *If $a_{ij} \leq 0$, for each $i \neq j$ and $a_{ii} > 0$, for each $i = 1, 2, \dots$, then one and only one of the following statements holds*

(i) $0 \leq \rho(\mathbf{T}_g) < \rho(\mathbf{T}_j) < 1$;

(ii) $1 \leq \rho(\mathbf{T}_j) < \rho(\mathbf{T}_g)$;

(iii) $\rho(\mathbf{T}_j) = \rho(\mathbf{T}_g) = 0$;

(iv) $\rho(\mathbf{T}_j) = \rho(\mathbf{T}_g) = 1$.

7.4 Error Bounds and Iterative Refinement

定理 7.4.1 Suppose that $\tilde{\mathbf{x}}$ is an approximation to the solution of $\mathbf{Ax} = \mathbf{b}$. \mathbf{A} is nonsingular matrix and \mathbf{r} is the residual vector for $\tilde{\mathbf{x}}$ ($\mathbf{r} = \mathbf{b} - \mathbf{A}\tilde{\mathbf{x}}$). Then for any natural norm

$$\|\mathbf{x} - \tilde{\mathbf{x}}\| = \|\mathbf{A}^{-1}\mathbf{r}\| \leq \|\mathbf{r}\|\|\mathbf{A}^{-1}\|$$

and if $\mathbf{x} \neq \mathbf{0}$ and $\mathbf{b} \neq \mathbf{0}$

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq \frac{\|\mathbf{A}\|\|\mathbf{A}^{-1}\|}{\|\mathbf{b}\|} \|\mathbf{r}\| \quad \text{with } \|\mathbf{b}\| \leq \|\mathbf{A}\|\|\mathbf{x}\|$$

7.4.1 Condition Numbers

定义 7.4.1 (Condition Number) The condition number of the nonsingular matrix \mathbf{A} relative to a norm $\|\cdot\|$ is

$$1 \leq \|\mathbf{I}\| \leq \|\mathbf{A}\mathbf{A}^{-1}\| \leq \|\mathbf{A}\|\|\mathbf{A}^{-1}\| = \mathbf{K}(\mathbf{A}).$$

A matrix \mathbf{A} is well-conditioned if $K(\mathbf{A})$ is close to 1, and is ill-conditioned when $K(\mathbf{A})$ is significantly greater than 1.

7.4.2 Iterative Refinement(迭代改善法)

设 $\mathbf{Ax} = \mathbf{b}$, 其中 $\mathbf{A} \in \mathbb{R}^{n \times n}$ 为非奇异矩阵, 且为病态方程组 (但不过分病态)。当求得线性方程组的近似解 \mathbf{x}_1 , 下面研究改善方程组近似解 \mathbf{x}_1 精度的方法。

首先用选主元三角分解法实现分解计算

$$\mathbf{PA} = \mathbf{LU}.$$

计算剩余向量

$$\mathbf{r}_1 = \mathbf{b} - \mathbf{Ax}_1,$$

求解 $\mathbf{Ad} = \mathbf{r}_1$, 得到的解记为 \mathbf{d}_1 。然后改善

$$\mathbf{x}_2 = \mathbf{x}_1 + \mathbf{d}_1.$$

在实际计算中, 由于有舍入误差, \mathbf{x}_2 只是方程组的近似解, 重复上述过程, 就产生一系列近似解序列 $\{\mathbf{x}_k\}$, 有时可能得到比较好的近似。