Numerical Analysis

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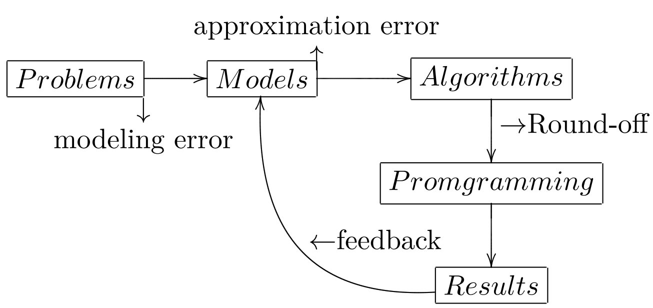
0.1　Preface



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：

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

$$\begin{cases} S:\ 0/1 & signpart \\ c:\ 11\,digits & exponential\ part. \\ f:\ 52\,digits & mantissa\ part \end{cases}$$

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

$\pm 0.d_1 d_2 \cdots d_n \times 10^n$ 其中 $1 \le d_1 \le 9$，$0 \le d_i \le 9$，$\forall i \ge 2$。如果记真实的数为 y，其浮点数表示为 $fl(y)$。

当存在 $y = 0.d_1 d_2 \cdots d_k d_{k+1} \cdots \times 10^n$，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 $p^\star$ is an approximation of p.*

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

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

$$\frac{|p - p^\star|}{p} \le 5 \times 10^{-t}$$

.

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）

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

Rounding:（其有效位数至少为 k）

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

Machine Operators

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

$$x\,\text{op}\,y = fl(fl(x)\,\text{op}\,fl(y))$$

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 : $a_0, a_1, \cdots, a_n(given); x$
output: $P_n(x)$

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

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

```

```python
    Args:
        poly: List, store the coefficient of the polynomial.
        x: Float, specify the variable in the polynomial.

    Returns:
        Float, result.

    Raises:
        If `poly' is empty, raise IndexError.
        If type(args) does not correspond, raise TypeError.
    """
    result = poly[0]
    for i in range(1, poly.__len__()):
        result = x*result + poly[i]
    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 $n \to \infty$，$\alpha_n \to \alpha$，$\beta_n \to 0$，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* $f \in [a,b]$, $\forall k \in f([a,b])$, $\exists c \in [a,b]$，$s.t.\ f(c) = k$。

```
def Bisection(fun, a:float, b:float, max_step:int=128, ...
    eps:float=1e-6)->float:
    mid_last = a
    if fun(a)*fun(b) < 0:
        for i in range(0, max_step):
            mid = (a+b) / 2
            if abs(mid-mid_last)<eps or abs(fun(mid))<eps:
                print("Step: %d\nZero: %fc"%(i, mid))
                return mid
            else:
                if fun(mid)*fun(a)<0:
                    b = mid
                else:
                    a = mid
            mid_last = mid
        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 $\exists$ *root* $P \in [a,b]$，则有 $|P_n - P| \le \frac{b-a}{x^n}$。

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

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

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 $g'(x) \le \kappa < 1$。

[Proof]
存在性：

$$\begin{cases} h(a) = & g(a) - a \ge 0 \\ h(b) = & g(b) - b \le 0 \end{cases}$$

于是有 $h(a)h(b) \le 0$，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 $P_1 \ne P_2$。

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

□

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 $|g'(x)|\le\kappa<1$。$\forall P_0\in[a,b]$，定义序列 $P_i=g(P_{i-1}),\quad i=1,2,\cdots$，则 $\lim_{n\to\infty}P_n=P$（P 为不动点）。

[Proof]

$$\begin{aligned}
|P_n-P| &= |g(P_{n-1}-g(P))| \\
&= |g'(\xi_{n-1})|\,|P_{n-1}-P| \\
&\le \kappa\,|P_{n-1}-P| \\
&\le \cdots \le \cdots \\
&\le \kappa^n\,|P_0-P| \to 0.
\end{aligned}$$

□

其中，寻找不动点的代码如下：

```
def fixed_point(fun, start:float=0, max_step:int=128, ...
    eps:float=1e-6)->float:
    new_val = fun(start)
    for i in range(0, max_step):
        old_val = new_val
        new_val = fun(old_val)
        if -eps<old_val-new_val<eps:
            print(i)
            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

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

并且有

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

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 $\{p_n\}_{n=0}^{\infty}$,

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

```
def Newton_method(f, df, start:float=0.0, max_step:int=32,...
    sign_dig:int=6)->float:
    fun = lambda x: x - f(x)/df(x)
    return fixed_point(fun, start, max_step, sign_dig)

def fixed_point(fun, start:float, max_step:int,...
    sign_dig:int)->float:
    fl = lambda x: round(x, 100)
    eps = 10**(-sign_dig)
    new_val = fun(start)
    for i in range(0, max_step):
        old_val = fl(new_val)
```

```
        new_val = fl(fun(old_val))
        if abs(old_val-new_val)<=2*eps:
            return (i, new_val)
    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.

```python
def false_position(f, start:list, max_step:int=32, ...
    eps:float=1e-6) -> float:
    """
    False position.
    ----------------------------
    Args:
        f: Function.
        start: List of float, the first iteration point.
        max_step: Integer, max number of iteration.

    Returns:
        Float zero.
        zero | fun(zero)\\sim 0.

    Raises:
        None.
    """
    p = [i    for i in start]
    q = [f(i) for i in start]
    for i in range(max_step):
        _p = p[-1] - q[-1]*(p[-1]-p[0])/(q[-1]-q[0])
        if abs(_p-p[-1]) < eps:
            return (i, _p)
        _q = f(_p)
        if _q*q[-1] < 0:
            p[0] = p[-1]
            q[0] = q[-1]
        p[-1] = _p
        q[-1] = _q
    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：

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

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*

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

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

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

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

[Proof]

$$p_{n+1} - p = g(p_n) - g(p) = g'(\xi_n)(p_n - p),$$
$$\Rightarrow \lim_{n\to\infty} \frac{p_{n+1} - p}{p_n - p} = \lim_{n\to\infty} g'(\xi_n) = g'(p)$$

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

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]

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

$\square$

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*

$$f(x_k) = P(x_k) \quad fork = 0 : n$$

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

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

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

[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

$$0 = g^{(n+1)}(\xi) = f^{(n+1)}(\xi) - P^{(n+1)}(\xi) - [f(x) - P(x)] \frac{\mathrm{d}^{n+1}}{\mathrm{d}t^{n+1}} \left[\prod_{i=0}^{n} \frac{(t - x_i)}{x - x_i} \right]_{t=\xi}$$

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

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

□

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 $x_{m_1}, x_{m_2}, \cdots, x_{m_k}$ is denoted $P_{m_1, m_2, \cdots m_k}(x)$.*

定理 3.2.1 *Let f be defined at $x_0, x_1, \cdots, x_k$, then*

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

is the kth 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 $x_{i-j}, \cdots, x_i$.

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

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 kth divided difference relative to $x_i, \cdots, x_{i+k}$ is

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

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

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

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.*

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

[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. $g^{(n)}(\xi) = 0$.

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

□

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

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

3.3.2 Forward Differences

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

In general,

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

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,

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

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

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

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}	$f[x_{-2}]$	$f[x_{-2}, x_{-1}]$	$f[x_{-2}, x_{-1}, x_0]$	$\underline{f[x_{-2}, x_{-1}, x_0, x_1]}$	$\underline{f[x_{-2}, x_{-1}, x_0, x_1, x_2]}$
x_{-1}	$f[x_{-1}]$	$\underline{f[x_{-1}, x_0]}$	$\underline{f[x_{-1}, x_0, x_1]}$	$\underline{f[x_{-1}, x_0, x_1, x_2]}$	
x_0	$\underline{f[x_0]}$	$\underline{f[x_0, x_1]}$	$f[x_0, x_1, x_2]$		
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 $M = \sum_{i=0}^{n} m_i + n$.

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

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

3.4.1 Hermite Polynomials

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

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

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

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 $x_0, \cdots, x_n$ are given together with values of f and f'. Define a new sequence $z_0, \cdots, z_{2n+1}$ by

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

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

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

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. $\begin{cases} \textit{natural boundary:} & S''(x_0) = S''(x_n) = 0. \\ \textit{clamped boundary:} & S'(x_0) = f'(x_0),\ S'(x_n) = f'(x_n). \end{cases}$

3.5.1 Construction of a Cubic Spline

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

(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:

$Ax = b$

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

Then we will get b_j, d_j by

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

3.5.2 Clamped Splines

$$Ax = b$$

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

第四章 Numerical Differentiation and Integration

4.1 Numerical Differentiation

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

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

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) *$\{x_0, x_1, \ldots, x_n\}$ are $(n+1)$ dis-*

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

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \prod_{k=0}^{n}\left(\frac{x-x_k}{k+1}\right) f^{(n+1)}(\xi(x)).$$

$$\Rightarrow f'(x) = \sum_{k=0}^{n} f(x_k)L_k'(x) + D_x\left[\prod_{k=0}^{n}\left(\frac{x-x_k}{k+1}\right)\right] f^{(n+1)}(\xi(x))$$
$$+ \prod_{k=0}^{n}\left(\frac{x-x_k}{k+1}\right) D_x\left[f^{(n+1)}(\xi(x))\right].$$

$$\Rightarrow f'(x_j) = \sum_{k=0}^{n} f(x_k)L_k'(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!}\prod_{\substack{k=0\\k\neq j}}^{n}(x_j - x_k).$$

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
$$f'(x_0) = \frac{1}{12h}\left[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h)\right.$$
$$\left. - f(x_0+2h)\right] + \frac{h^4}{30}f^{(5)}(\xi).$$

- Five-Point Endpoint Formula
$$f'(x_0) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h)\right.$$
$$\left. +16f(x_0+3h - 3f(x_0+4h))\right] + \frac{h^4}{5}f^{(5)}(\xi).$$

4.1.3 Second Derivative Midpoint Formula

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

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

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

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

$$f(x_0+h) = \tilde{f}(x_0+h)+e(x_0+h) \qquad \textit{and} \qquad f(x_0-h) = \tilde{f}(x_0-h)+e(x_0-h)$$

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 $O(h)$

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

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

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

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

4.3 Elements of Numerical Integration

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

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

4.3.1 The Trapezoidal Rule

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

$$\begin{aligned}
\int_a^b f(x)\mathrm{d}x &= \int_a^b \left[\frac{(x - x_0)}{(x_1 - x_0)f(x_1)} + \frac{(x - x_1)}{(x_0 - x_1)f(x_0)}\right]\mathrm{d}x + \frac{1}{2}\int_a^b (x - x_0)(x - x_1)f''(\xi(x))\mathrm{d}x \\
&= \int_{x_0}^{x_1} \frac{(x - x_0)f(x_1) - (x - x_1)f(x_0)}{x_1 - x_0}\mathrm{d}x + \frac{f''(\xi)}{2}\left[\frac{x^3}{3} - \frac{(x_0 + x_1)}{2}x^2 + x_0x_1x\right]_{x_0}^{x_1} \\
&= \left[\frac{(x - x_0)^2 f(x_1) - (x - x_1)^2 f(x_0)}{2(x_0 - x_1)}\right]_{x_0}^{x_1} - \frac{h^3}{12}f''(\xi) \\
&= \frac{h}{2}\left[f(x_0) + f(x_1)\right] - \frac{h^3}{12}f''(\xi).
\end{aligned}$$

4.3.2 Simpson's Rule

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

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 $k = 0, 1, \ldots, n$.

4.3.4 New-tom-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 $i = 0, 1, \ldots, n$, where $x_0 = a$, $x_n = b$ and $h = (b-a)/n$.

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

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

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

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

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

n=1 Trapezoidal rule

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

n=2 Simpson's rule

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

n=3 Simpson's Three-Eighths rule

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

n=4

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

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

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

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

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

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

n=0 Midpoint rule

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

n=1

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

n=2

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

n=3

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

4.4 Composite Numerical Integration

To calculate an aribitrary integral $\int_a^b f(x)\mathrm{d}x$, 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 $j = 0, 1, \ldots, n$, we have

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

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 $j = 0, 1, \ldots, n$. There exists a $\mu \in (a,b)$ s.t. with n subintervals*

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

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 $j = 0, 1, \ldots, n$. There exists a $\mu \in (a,b)$ s.t. with n subintervals*

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

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 $j = -1, 0, \ldots, n+1$. There exists a $\mu \in (a,b)$ s.t. with $n+2$ subintervals*

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

4.4.1 Round-off Error Stability

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

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 $i = 2, \ldots, n$ do Steps 4–8.

Step 4 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 $j = 2, \ldots, i$

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

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

Step 7 Set $h = h/2$.

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

Step 9 STOP.

4.6 Gaussian Quadrature

4.6.1 Legendre Polynomial

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

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

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

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

[Proof]

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

$$\int_{-1}^{1} P(x)\mathrm{d}x = \int_{-1}^{1}\sum_{i=1}^{n} P(x_i)L_i(x)\mathrm{d}x = \int_{-1}^{1}\sum_{i=1}^{n}\prod_{\substack{j=1 \\ j\neq i}}^{n}\left(\frac{x - x_j}{x_i - x_j}\right)P(x_i)\mathrm{d}x$$

$$= \sum_{i=1}^{n}\left[\int_{-1}^{1}\prod_{\substack{j=1 \\ j\neq i}}^{n}\left(\frac{x - x_j}{x_i - x_j}\right)\mathrm{d}x\right]P(x_i) = \sum_{i=1}^{n} C_i P(x_i).$$

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

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

$\square$

4.6.2 Gaussian Quadrature on Arbitrary Intervals

An integral $\int_a^b f(x)\mathrm{d}x$ over an arbitrart $[a, b]$ can be transformed into an integral over $[-1, 1]$

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

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* Lispschitz 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*

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

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*

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

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

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

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

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

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

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 $i = 1, 2, \cdots, N$, by deleting the remainder term, then Euler's method is

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

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*

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

and that a constant M exists with

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

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

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha$$

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

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

[Proof]

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

□

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

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

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*

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

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

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

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

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

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha$$

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

[Proof]

$$y_{i+1} = y_i + hf(t_i, y_i) + \cdots + \frac{h^n}{n!} f^{(n-1)}(t_i, y_i) + \frac{h^{n+1}}{(n+1)!} f^{(n)}(\xi_i, y(\xi_i))$$

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

for each $i = 0, 1, \cdots, N-1$. 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 $i = 1, 2, \cdots, N$. $\square$

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 $D = \{(t, y) | a \le t \le b, c \le y \le d\}$ ($D = [a, b] \times [c, d]$) 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

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

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

The function $P_n(t,y)$ is called the nth 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

$$\begin{cases} y_{n+1} = y_n + h(c_1k_1 + c_2k_2) \\ k1 = f(x_n,y_n) \\ k1 = f(x_n+\lambda_2 h, y_n + \mu_{21}hk_1) \end{cases}$$

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

5.4.2 Midpoint Method

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

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

5.4.3 Modified Euler Method

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

5.4.4 Higher-Order Runge-Kutta Methods

Runge-Kutta Order Three:

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

Runge-Kutta Order Four:

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

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 $h \to 0$ 时有 $y_n \to y(x_n)$，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*

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

*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)

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

所以有

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

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

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

再注意到当 $x_n-x_0=nh\leq T$ 时，

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

最终有

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

由此可以断定，如果初值准确，即 $e_0=0$，证毕。 □

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*

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

] 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:

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

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.

$$\begin{cases} \textit{When } b_m = 0, \textit{ the method is called explicit, or open.} \\ \textit{When } b_m \neq 0, \textit{ the method is called implicit, or closed.} \end{cases}$$

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

$$
\begin{aligned}
E1 :& a_{11}x_1 + a12x_2 + \cdots + a_{1n}x_n = a_{1,n+1} \\
E2 :& a_{21}x_1 + a22x_2 + \cdots + a_{2n}x_n = a_{2,n+1} \\
&\vdots \\
En :& a_{n1}x_1 + an2x_2 + \cdots + a_{nn}x_n = a_{n,n+1}
\end{aligned}
$$

6.1.2 Operation Counts

Multiplications / divisions

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

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

```
def gaussian_elimination_partial_pivoting(A, b):
    np_result = A**-1 * b
    print(np_result.T)
    n = A.shape[0]
    x = np.zeros((n,1))
    tmp = 0
    for k in range(n-1):
        M = k
        for m in range(k+1,n):
            if A[m,k] > A[M,k]: M = m
        A[[k,M]] = A[[M,k]]
        b[[k,M]] = b[[M,k]]
        for i in range(k+1,n):
            m = A[i,k] / A[k,k]
            for j in range(k,n):
                A[i,j] = A[i,j] - m*A[k,j]
            b[i,0] = b[i,0] - m*b[k,0]
```

```
    x[-1,0] = b[-1,0] / A[-1,-1]
    for i in range(n-2,-1,-1):
        for j in range(i+1,n):
            tmp += A[i,j] * x[j,0]
        x[i,0] = (b[i,0] - tmp) / A[i,i]
        tmp = 0
    return x
```

6.1.6 Gaussian Elimination with Scaled Partial Pivoting

```
def gaussian_elimination_scaled_partial_pivoting(A, b):
    np_result = A**-1 * b
    print(np_result.T)
    n = A.shape[0]
    x = np.zeros((n,1))
    tmp = 0
    for k in range(n):
        M = np.max(A[k,:])
        A[k,:] /= M
        b[k,0] /= M
    for k in range(n-1):
        for i in range(k+1,n):
            m = A[i,k] / A[k,k]
            for j in range(k,n):
                A[i,j] = A[i,j] - m*A[k,j]
            b[i,0] = b[i,0] - m*b[k,0]
    x[-1,0] = b[-1,0] / A[-1,-1]
    for i in range(n-2,-1,-1):
        for j in range(i+1,n):
            tmp += A[i,j] * x[j,0]
        x[i,0] = (b[i,0] - tmp) / A[i,i]
        tmp = 0
    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 maxtrix L and an upper-triangular matrix U, that is $A = LU$, where $m_{ji} = a_{ji}^{(i)}/a_{ii}^{(i)}$*

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

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) $\|\mathbf{x}\| \geq \mathbf{0}$ *for all* $\mathbf{x} \in \mathbb{R}^{\mathbf{n}}$.

(ii) $\|\mathbf{x}\| = \mathbf{0}$ *if and only if* $\mathbf{x} = \mathbf{0}$.

(iii) $\|\alpha\mathbf{x}\| = |\alpha|\,\|\mathbf{x}\|$ *for all* $\alpha \in \mathbb{R}$ *and* $\mathbf{x} \in \mathbb{R}^{\mathbf{n}}$.

(iv) $\|\mathbf{x}+\mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$ *for all* $\mathbf{x}, \mathbf{y} \in \mathbb{R}^{\mathbf{n}}$.

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

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

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

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

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 s a real-valued function, $\|\cdot\|$, defined on this ser, satisfying for all $n \times n$ matrices $\mathbf{A}$ and $\mathbf{B}$ and all real numbers α.*

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

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

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

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

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

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

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

is a matrix norm.

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

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

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*

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

(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) $\|\mathbf{A}\|_{\mathbf{1}} = \max_{\mathbf{j}} \sum_{\mathbf{i=1}}^{\mathbf{n}} |\mathbf{a_{ij}}|$,*(列和最大)*

(ii) $\|\mathbf{A}\|_{\mathbf{2}} = [\rho(\mathbf{A^t A})]^{\mathbf{1/2}}$,

(iii) $\|\mathbf{A}\|_{\infty} = \max_{\mathbf{i}} \sum_{\mathbf{j=1}}^{\mathbf{n}} |\mathbf{a_{ij}}|$,*(行和最大)*

(iv) $\rho(\mathbf{A}) \le \|\mathbf{A}\|$*, 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*

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

定理 7.2.2 *The following statements are equivalent*

(i) $\mathbf{A}$ *is a convergent matrix.*

(ii) $\lim_{n\to\infty} \|\mathbf{A^n}\| = \mathbf{0}$*, for some natural norm.*

(iii) $\lim_{n\to\infty} \|\mathbf{A^n}\| = \mathbf{0}$*, for all natural norms.*

(iv) $\rho(\mathbf{A}) < \mathbf{1}$.

(v) $\lim_{n\to\infty} \mathbf{A^n x} = \mathbf{0}$*, 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 ith equation in $A\mathbf{x} = \mathbf{b}$ for x_i to obtain(provided $a_{ii} \neq 0$)

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

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 $x^{(0)}$ is selected, the sequence of approximate solution vectors is generated by computing

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

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

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

7.3.2 The Gauss-Seidel Method

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

That is

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

Then

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

7.3.3 General Iterative Methods

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

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

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

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

定理 7.3.1 *For any* $x^{(0)} \in \mathbb{R}^n$, *the sequence* $\left\{x^{(k)}\right\}_{k=0}^{\infty}$ *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* $\|\mathbf{T}\| < \mathbf{1}$ *for any natural matrix*

(i)

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

(ii)

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

定理 7.3.2 (Stein-Rosenberg) *If* $a_{ij} \leq 0$, *for each* $i \neq j$ *and* $a_{ii} > 0$, *for each* $i = 1, 2, \ldots$, *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) $\rho(\mathbf{T}_j) = \rho(\mathbf{T}_j) = 0$;

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