

# Document for MTK

Zeyu Wang<sup>1</sup>

May 06, 2024

---

<sup>1</sup>Email: zeyu.wang.0117@outlook.com

# Contents

1	Polynomial .....	1
1.1	Single Variable Polynomial .....	1
1.2	Orthogonal Polynomial .....	1
1.2.1	Legendre polynomial .....	1
1.2.2	Chebyshev polynomial of the first kind .....	2
1.2.3	Chebyshev polynomial of the second kind .....	2
1.2.4	Laguerre polynomial .....	2
1.2.5	Hermite polynomial (probability theory form) .....	3
2	Interpolation .....	4
2.1	Polynomial Interpolation .....	4
2.1.1	Lagrange formula .....	4
2.1.2	Newton formula .....	4
2.1.3	Neville-Aitken algorithm .....	4
2.1.4	Hermite interpolation .....	5
2.1.5	Approximation .....	5
2.1.6	Error analysis .....	6
2.2	Spline .....	6
2.2.1	Cubic spline .....	6
2.2.2	B-spline .....	7
2.2.3	Error analysis .....	7
3	Integration .....	8
3.1	Newton-Cotes Formulas .....	8
3.1.1	Midpoint rule .....	8
3.1.2	Trapezoidal rule .....	9
3.1.3	Simpson's rule .....	9
3.2	Gauss Formulas .....	9
4	Optimization .....	10
4.1	One-dimensional Line Search .....	10
4.2	Unconstrained Optimization .....	11
5	Initial Value Problem .....	13
5.1	Linear Multistep Method .....	13
5.2	Runge-Kutta Method .....	13
5.3	Theoretical analysis .....	14
5.3.1	Error analysis .....	14
5.3.2	Stability .....	14
5.3.3	Convergence .....	15
5.4	Important Methods .....	15
5.4.1	Forward Euler's method .....	15
5.4.2	Backward Euler's method .....	16
5.4.3	Trapezoidal method .....	16
5.4.4	Midpoint method (Leapfrog method) .....	16

5.4.5	Heun's third-order RK method .....	16
5.4.6	Classical fourth-order RK method .....	16
5.4.7	TR-BDF2 method .....	17
6	Number Theory .....	18
6.1	Prime Number .....	18
6.1.1	Primality testing .....	18
6.1.2	Sieves .....	18

# Chapter 1

## Polynomial

### 1.1 Single Variable Polynomial

**Definition 1.1.** Denoted by  $\mathbb{V}$  a linear space and  $x$  the variable, a **(single variable) polynomial** over  $\mathbb{V}$  is defined as

$$p_{n(x)} = \sum_{i=0}^n c_i x^i,$$

where  $c_0, \dots, c_n \in \mathbb{V}$  are constants that called the **coefficients of the polynomial**.

**Definition 1.2.** Given a polynomial  $p(x) = \sum_{i=0}^n c_i x^i$  where  $c_n \neq 0$ , the degree of  $p(x)$  is marked as  $\deg(p(x)) = n$ . In particular, the degree of zero polynomial  $p(x) = 0$  is  $\deg(0) = -\infty$ .

**Theorem 1.3.** Denoted by  $\mathbb{P}_n = \{p : \deg(p) \leq n\}$  the set of polynomials with degree no more than  $n$  ( $n \geq 0$ ), and  $\mathbb{P} = \bigcup_{n=0}^{\infty} \mathbb{P}_n$  the set contains all polynomials, then  $\mathbb{P}_n$  is a linear space and satisfies

$$\{0\} = \mathbb{P}_0 \subset \mathbb{P}_1 \subset \dots \subset \mathbb{P}_n \subset \dots \subset \mathbb{P}$$

### 1.2 Orthogonal Polynomial

**Definition 1.4.** Given a weight function  $\rho(x) : [a, b] \rightarrow \mathbb{R}^+$ , satisfies

$$\int_a^b \rho(x) dx > 0, \int_a^b x^k \rho(x) dx > 0 \text{ exists.}$$

The set of **orthogonal polynomials** on  $[a, b]$  with the weight function  $\rho(x)$  is defined as

$$\{p_i, i \in \mathbb{N}\} \subset L_\rho([a, b]) = \left\{ f(x) : \int_a^b f^2(x) \rho(x) dx < \infty \right\}.$$

where  $\{p_i, i \in \mathbb{N}\}$  are calculate from  $\{x^n, n \in \mathbb{N}\}$  using the Gram-Schmidt process with the inner product

$$\forall f, g \in L_\rho([a, b]), \langle f, g \rangle = \int_a^b \rho(x) f(x) g(x) dx.$$

**Theorem 1.5.** Orthogonal polynomials  $p_{n-1}(x), p_n(x), p_{n+1}(x)$  satisfies

$$p_{n+1}(x) = (a_n + b_n x) p_n(x) + c_n p_{n-1}(x).$$

where  $a_n, b_n, c_n$  are depends on  $[a, b]$  and  $\rho$ .

**Theorem 1.6.** The orthogonal polynomial  $p_n(x)$  on  $[a, b]$  with the weight function  $\rho(x)$  has  $n$  roots on  $(a, b)$ .

#### 1.2.1 Legendre polynomial

**Definition 1.7.** The **Legendre polynomial** is defined on  $[-1, 1]$  with the weight function  $\rho(x) = 1$ .

**Theorem 1.8.** The Legendre polynomials  $\{p_i(x), i \in \mathbb{N}\}$  satisfies

$$\int_{-1}^1 p_i(x)p_j(x)dx = \begin{cases} \frac{2}{2i+1}, & i = j \\ 0, & i \neq j. \end{cases}$$

**Theorem 1.9.** The Legendre polynomial  $p_{n-1}, p_n, p_{n+1}$  satisfies

$$p_{n+1}(x) = \frac{2n+1}{n+1}xp_n(x) - \frac{n}{n+1}p_{n-1}(x).$$

**Example 1.10.** The first three terms of Legendre polynomials is

$$p_0(x) = 1, \quad p_1(x) = x, \quad p_2(x) = \frac{3}{2}x^2 - \frac{1}{2}.$$

### 1.2.2 Chebyshev polynomial of the first kind

**Definition 1.11.** The **Chebyshev polynomial of the first kind** is defined on  $[-1, 1]$  with the weight function  $\rho(x) = \frac{1}{\sqrt{1-x^2}}$ .

**Theorem 1.12.** The Chebyshev polynomials of the first kind  $\{p_i(x), i \in \mathbb{N}\}$  satisfies

$$\int_{-1}^1 \frac{1}{\sqrt{1-x^2}} p_i(x)p_j(x)dx = \begin{cases} \pi & i = j = 0 \\ \frac{\pi}{2} & i = j \neq 0 \\ 0 & i \neq j. \end{cases}$$

**Theorem 1.13.** The Chebyshev polynomial of the first kind  $p_{n-1}, p_n, p_{n+1}$  satisfies

$$p_{n+1}(x) = 2xp_n(x) - p_{n-1}(x).$$

**Example 1.14.** The first three terms of Chebyshev polynomials of the first kind is

$$p_0(x) = 1, \quad p_1(x) = x, \quad p_2(x) = 2x^2 - 1.$$

### 1.2.3 Chebyshev polynomial of the second kind

**Definition 1.15.** The **Chebyshev polynomial of the second kind** is defined on  $[-1, 1]$  with the weight function  $\rho(x) = \sqrt{1-x^2}$ .

**Theorem 1.16.** The Chebyshev polynomials of the second kind  $\{p_i(x), i \in \mathbb{N}\}$  satisfies

$$\int_{-1}^1 \sqrt{1-x^2} p_i(x)p_j(x)dx = \begin{cases} \frac{\pi}{2}, & i = j \\ 0, & i \neq j. \end{cases}$$

**Theorem 1.17.** The Chebyshev polynomial of the second kind  $p_{n-1}, p_n, p_{n+1}$  satisfies

$$p_{n+1}(x) = 2xp_n(x) - p_{n-1}(x).$$

**Example 1.18.** The first three terms of Chebyshev polynomials of the second kind is

$$p_0(x) = 1, \quad p_1(x) = 2x, \quad p_2(x) = 4x^2 - 1.$$

### 1.2.4 Laguerre polynomial

**Definition 1.19.** The **Laguerre polynomial** is defined on  $[0, +\infty)$  with the weight function  $\rho(x) = x^\alpha e^{-x}$ .

**Theorem 1.20.** The Laguerre polynomial  $\{p_i(x), i \in \mathbb{N}\}$  satisfies

$$\int_0^{+\infty} x^\alpha e^{-x} p_i(x) p_j(x) dx = \begin{cases} \frac{\Gamma(n+\alpha+1)}{n!}, & i = j \\ 0, & i \neq j. \end{cases}$$

**Theorem 1.21.** For  $\alpha = 0$ , the Laguerre polynomial  $p_{n-1}, p_n, p_{n+1}$  satisfies

$$p_{n+1}(x) = (2n+1-x)p_n(x) - n^2 p_{n-1}(x).$$

**Example 1.22.** For  $\alpha = 0$ , the first three terms of Laguerre polynomial is

$$p_0(x) = 1, \quad p_1(x) = -x + 1, \quad p_2(x) = x^2 - 4x + 2.$$

### 1.2.5 Hermite polynomial (probability theory form)

**Definition 1.23.** The **Hermite polynomial** is defined on  $(-\infty, +\infty)$  with the weight function  $\rho(x) = \left(\frac{1}{\sqrt{2\pi}}\right)e^{-\frac{x^2}{2}}$ .

**Theorem 1.24.** The Hermite polynomial  $\{p_i(x), i \in \mathbb{N}\}$  satisfies

$$\int_0^{+\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} p_i(x) p_j(x) dx = \begin{cases} n!, & i = j \\ 0, & i \neq j. \end{cases}$$

**Theorem 1.25.** For  $\alpha = 0$ , the Hermite polynomial  $p_{n-1}, p_n, p_{n+1}$  satisfies

$$p_{n+1}(x) = xp_n(x) - np_{n-1}(x).$$

**Example 1.26.** For  $\alpha = 0$ , the first three terms of Hermite polynomial is

$$p_0(x) = 1, \quad p_1(x) = x, \quad p_2(x) = x^2 - 1.$$

# Chapter 2

## Interpolation

### 2.1 Polynomial Interpolation

#### 2.1.1 Lagrange formula

**Definition 2.1.** To interpolate given points  $(x_0, f(x_0)), \dots, (x_n, f(x_n))$ , the Lagrange formula is

$$p_n(x) = \sum_{i=0}^n f(x_i) l_i(x),$$

where the **elementary Lagrange interpolation polynomial** (or **fundamental polynomial**) for pointwise interpolation  $l_k(x)$  is

$$l_k(x) = \prod_{i=0, i \neq k}^n \frac{x - x_i}{x_k - x_i}.$$

In particular, for  $n = 0, l_0(x) = 1$ .

#### 2.1.2 Newton formula

**Definition 2.2.** The  $k$ th divided difference ( $k \in \mathbb{N}^+$ ) on the **table of divided differences**

$$\begin{array}{l|llll} x_0 & f[x_0] & & & \\ x_1 & f[x_1] & f[x_0, x_1] & & \\ x_2 & f[x_2] & f[x_1, x_2] & f[x_0, x_1, x_2] & \\ x_3 & f[x_3] & f[x_2, x_3] & f[x_1, x_2, x_3] & f[x_0, x_1, x_2, x_3] \\ \dots & \dots & \dots & \dots & \dots \end{array}$$

where the **divided differences** satisfy

$$\begin{aligned} f[x_0] &= f(x_0), \\ f[x_0, \dots, x_k] &= \frac{f[x_1, \dots, x_k] - f[x_0, \dots, x_{k-1}]}{x_k - x_0}. \end{aligned}$$

**Corollary 2.3.** Suppose  $(i_0, \dots, i_k)$  is a permutation of  $(0, \dots, k)$ . Then

$$f[x_0, \dots, x_k] = f[x_{i_0}, \dots, x_{i_k}].$$

**Theorem 2.4.** For distinct points  $x_0, \dots, x_n$  and  $x$ , we have

$$f(x) = f[x_0] + f[x_0, x_1](x - x_0) + \dots + f[x_0, \dots, x_n] \prod_{i=0}^{n-1} (x - x_i) + f[x_0, \dots, x_n, x] \prod_{i=0}^n (x - x_i).$$

**Definition 2.5.** The **Newton formula** for interpolating the points  $(x_0, f(x_0)), \dots, (x_n, f(x_n))$  is

$$p_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + \dots + f[x_0, \dots, x_n] \prod_{i=0}^{n-1} (x - x_i).$$

#### 2.1.3 Neville-Aitken algorithm

**Definition 2.6.** Denote  $p_0^{[i]}(x) = f(x_i)$  for  $i = 0, \dots, n$ . For all  $k = 0, \dots, n-1$  and  $i = 0, \dots, n-k-1$ , define

$$p_{k+1}^{[i]}(x) = \frac{(x - x_i)p_k^{[i+1]}(x) - (x - x_{i+k+1})p_k^{[i]}(x)}{x_{i+k+1} - x_i}.$$

Then each  $p_k^{[i]}(x)$  is the interpolating polynomial for the function  $f$  at the points  $x_i, \dots, x_{i+k}$ . In particular,  $p_n^{[0]}(x)$  is the interpolating polynomial of degree  $n$  for the function  $f$  at the points  $x_0, \dots, x_n$ .

### 2.1.4 Hermite interpolation

**Definition 2.7.** Given distinct points  $x_0, \dots, x_k$  in  $[a, b]$ , non-negative integers  $m_0, \dots, m_k$ , and a function  $f \in C^M[a, b]$  where  $M = \max_{i=0, \dots, k} (m_i)$ , the **Hermite interpolation problem** seeks a polynomial  $p(x)$  of the lowest degree satisfies

$$\forall i \in \{0, \dots, k\}, \forall \mu \in \{0, \dots, m_i\}, p^{(\mu)}(x_i) = f^{(\mu)}(x_i).$$

**Definition 2.8. (Generalized divided difference)** Let  $x_0, \dots, x_k$  be  $k+1$  pairwise distinct points with each  $x_i$  repeated  $m_i + 1$  times; write  $N = k + \sum_{i=0}^k m_i$ . The  $N$ th divided difference associated with these points is the coefficient of  $x^N$  in the polynomial  $p$  that uniquely solves the Hermite interpolation problem.

**Corollary 2.9.** The  $n$ th divided difference at  $n+1$  “confluent” (i.e. identical) points is

$$f[x_0, \dots, x_0] = \frac{1}{n!} f^{(n)}(x_0),$$

where  $x_0$  is repeated  $n+1$  times on the left-hand side.

### 2.1.5 Approximation

**Definition 2.10.** Given condition functions  $c_0, \dots, c_k : \mathbb{P}_n \rightarrow \mathbb{R}^+$ , the **Approximation problem** seeks a polynomial  $p_n(x)$  of the given degree  $n$  satisfies a unconstrained optimization

$$\min_{p_n \in \mathbb{P}_n} \sum_{i=0}^k c_i(p_n^{(m_i)}).$$

where condition function  $c(p)$  includes but is not limited to

$$|p^{(m)}(x)|, (p_n^{(m)}(x))^2, \int_a^b |p^{(m)}| \, dx, \int_a^b (p^{(m)})^2 \, dx.$$

**Example 2.11.** For non-negative integers  $m_0, \dots, m_k$  and condition functions  $c_i(p_n) = (p_n^{(m_i)}(x))^2$ , denote by

$$p_n(x) = \sum_{i=0}^n c_i x^i$$

the polynomial of the given degree  $n$ , then the  $m$ th derivative of  $p_n$  is

$$p_n^{(m)}(x) = \sum_{i=m}^n \frac{i!}{(i-m)!} c_i x^{i-m}.$$

All above implies the least squares system



$$\begin{cases} p_n^{(m_0)}(x) = \sum_{i=m_0}^n \frac{i!}{(i-m_0)!} c_i x^{i-m_0} = 0, \\ \dots \\ p_n^{(m_k)}(x) = \sum_{i=m_k}^n \frac{i!}{(i-m_k)!} c_i x^{i-m_k} = 0, \end{cases}$$

which can be solved by algorithms such as Householder transformation.

### 2.1.6 Error analysis

**Theorem 2.12.** Let  $f \in C^n[a, b]$  and suppose that  $f^{(n+1)}(x)$  exists at each point of  $(a, b)$ . Let  $p_n(x) \in \mathbb{P}_n$  denote the unique polynomial that coincides with  $f$  at  $x_0, \dots, x_n$ . Define

$$R_n(f; x) = f(x) - p_n(x),$$

as the **Cauchy remainder** of the polynomial interpolation.

If  $a \leq x_0 < \dots < x_n \leq b$ , then there exists some  $\xi \in (a, b)$  satisfies

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

where the value of  $\xi$  depends on  $x, x_0, \dots, x_n$  and  $f$ .

**Theorem 2.13.** For the Hermite interpolation problem, denote  $N = k + \sum_{i=0}^k m_i$ . Denote by  $p_N(x) \in \mathbb{P}_N$  the unique solution of the problem. Suppose  $f^{(N+1)}(x)$  exists in  $(a, b)$ . Then there exists some  $\xi \in (a, b)$  satisfies

$$R_N(f; x) = \frac{f^{(N+1)}(\xi)}{(N+1)!} \prod_{i=0}^k (x - x_i)^{m_i+1}.$$

## 2.2 Spline

**Definition 2.14.** Given nonnegative integers  $n, k$ , and a strictly increasing sequence  $a = x_1 < \dots < x_N = b$ , the set of **spline** functions of degree  $n$  and smoothness class  $k$  relative to the partition  $\{x_i\}$  is

$$\mathbb{S}_n^k = \left\{ s : s \in C^k[a, b]; \forall i \in \{1, \dots, N-1\}, s|_{[x_i, x_{i+1}]} \in \mathbb{P}_n \right\},$$

where  $x_i$  is the **knot** of the spline.

### 2.2.1 Cubic spline

**Definition 2.15. (Boundary conditions of splines)** The followings are common boundary conditions of cubic splines.

- The **complete cubic spline**  $s$  satisfies  $s'(a) = f'(a), s'(b) = f'(b)$ ;
- The **cubic spline with specified second derivatives**  $s$  satisfies  $s''(a) = f''(a), s''(b) = f''(b)$ ;
- The **natural cubic spline**  $s$  satisfies  $s''(a) = s''(b) = 0$ ;
- The **not-a-knot cubic spline**  $s$  satisfies  $s'''(x)$  exists at  $x = x_2$  and  $x = x_{N-1}$ .
- The **periodic cubic spline**  $s$  satisfies  $s(a) = s(b), s'(a) = s'(b), s''(a) = s''(b)$ .

**Theorem 2.16.** Denote  $m_i = s'(x_i), M_i = s''(x_i)$  for  $s \in \mathbb{S}_3^2$ , then

$$\forall i = 2, 3, \dots, N-1, \quad \lambda_i m_{i-1} + 2m_i + \mu_i m_{i+1} + 1 = 3\mu_i f[x_i, x_{i+1}] + 3\lambda_i f[x_{i-1}, x_i],$$

$$\forall i = 2, 3, \dots, N-1, \quad \mu_i M_{i-1} + 2M_i + \lambda_i m_{i+1} = 6f[x_{i-1}, x_i, x_{i+1}],$$

where

$$\mu_i = \frac{x_i - x_{i-1}}{x_{i+1} - x_{i-1}}, \quad \lambda_i = \frac{x_{i+1} - x_i}{x_{i+1} - x_{i-1}}.$$

In particular,  $m_i$  and  $M_i$  should be replaced to the derivatives given at the boundary.

**Theorem 2.17.** Cubic spline  $s \in \mathbb{S}_3^2$  from the linear system of  $\lambda_i, \mu_i, m_i, M_i$  and the boundary conditions.

## 2.2.2 B-spline

**Definition 2.18.** B-splines are defined recursively by

$$B_i^{n+1}(x) = (x - x_{i-1})(x_{i+n} - x_{i-1})B_i^n(x) + \frac{x_{i+n+1} - x}{x_{i+n+1} - x_{i-1}}B_{i+1}^n(x),$$

where recursion base is the B-spline of degree zero

$$B_i^0(x) = \begin{cases} 1, & x \in (x_{i-1}, x_i], \\ 0, & \text{otherwise.} \end{cases}$$

**Theorem 2.19.** The  $\{B_i^n(x)\}$  forms a basis of  $\mathbb{S}_n^{n-1}$ .

**Definition 2.20.** For  $N \in \mathbb{N}^*$ , the **support** of a  $B_i^n(x)$  is

$$\text{supp } \{B_i^n(x)\} = \overline{\{x \in \mathbb{R} : B_i^n(x) \neq 0\}} = [x_{i-1}, x_{i+n}].$$

**Theorem 2.21. (Integrals of B-splines)** The average of a B-spline over its support only depends on its degree,

$$\frac{1}{t_{i+n} - t_{i-1}} \int_{t_{i-1}}^{t_{i+n}} B_i^n(x) dx = \frac{1}{n+1}.$$

**Theorem 2.22. (Derivatives of B-splines)** For  $n \geq 2$ , we have

$$\forall x \in \mathbb{R}, \quad \frac{d}{dx} B_i^n(x) = \frac{nB_i^{n-1}(x)}{x_{i+n-1} - x_{i-1}} - \frac{nB_{i+1}^{n-1}(x)}{x_{i+n} - x_i}.$$

For  $n = 1$ , it holds for all  $x$  except  $x_{i-1}, t_i, t_{i+1}$ , where the derivative of  $B_i^1(x)$  is not defined.

## 2.2.3 Error analysis

**Theorem 2.23.** Suppose a function  $f \in C^4[a, b]$ , is interpolated by a complete cubic spline or a cubic spline with specified second derivatives at its end points. Then

$$\forall m = 0, 1, 2, |f^{(m)}(x) - s^{(m)}(x)| \leq c_m h^{4-m} \max_{x \in [a, b]} |f^{(4)}(x)|,$$

where  $c_0 = \frac{1}{16}, c_1 = c_2 = \frac{1}{2}$  and  $h = \max_{i=1, \dots, N-1} |x_{i+1} - x_i|$ .

# Chapter 3

## Integration

**Definition 3.1.** A **weighted quadrature formula**  $I_n(f)$  is a linear function

$$I_n(f) = \sum_{i=1}^n w_i f(x_i),$$

which approximates the integral of a function  $f \in C[a, b]$ ,

$$I(f) = \int_a^b \rho(x) f(x) dx,$$

where the weight function  $\rho \in [a, b]$  satisfies  $\forall x \in (a, b), \rho(x) > 0$ . The points  $\{x_i\}$  at which the integrand  $f$  is evaluated are called nodes or abscissas, and the multipliers  $\{w_i\}$  are called weights or coefficients.

**Definition 3.2.** A weighted quadrature formula has (polynomial) **degree of exactness**  $d_E$  iff

$$\forall f \in \mathbb{P}_{d_E}, \quad E_n(f) = 0,$$

$$\exists g \in \mathbb{P}_{d_E+1}, \text{ s.t. } E_n(g) \neq 0$$

where  $\mathbb{P}_d$  denotes the set of polynomials with degree no more than  $d$ .

**Theorem 3.3.** A weighted quadrature formula  $I_n(f)$  satisfies  $d_E \leq 2n - 1$ .

**Definition 3.4.** The **error** or **remainder** of  $I_n(f)$  is

$$E_n(f) = I(f) - I_n(f),$$

where  $I_n(f)$  is said to be convergent for  $C[a, b]$  iff

$$\forall f \in C[a, b], \quad \lim_{n \rightarrow +\infty} E_n(f) = 0.$$

**Theorem 3.5.** Let  $x_1, \dots, x_n$  be given as distinct nodes of  $I_n(f)$ . If  $d_E \geq n - 1$ , then its weights can be deduced as

$$\forall k \in \{1, \dots, n\}, w_k = \int_a^b \rho(x) l_k(x) dx,$$

where  $l_k(x)$  is the elementary Lagrange interpolation polynomial for pointwise interpolation applied to the given nodes.

### 3.1 Newton-Cotes Formulas

**Definition 3.6.** A **Newton-Cotes formula** is a formula based on approximating  $f(x)$  by interpolating it on uniformly spaced nodes  $x_1, \dots, x_n \in [a, b]$ .

#### 3.1.1 Midpoint rule

**Definition 3.7.** The **midpoint rule** is a formula based on approximating  $f(x)$  by the constant  $f\left(\frac{a+b}{2}\right)$ .

For  $\rho(x) \equiv 1$ , it is simply

$$I_M(f) = (b - a) f\left(\frac{a + b}{2}\right).$$

**Theorem 3.8.** For  $f \in C^2[a, b]$ , with weight function  $\rho \equiv 1$ , the error (remainder) of midpoint rule satisfies

$$\exists \xi \in [a, b], \text{ s.t. } E_M(f) = \frac{(b-a)^3}{24} f''(\xi).$$

**Corollary 3.9.** The midpoint rule has  $d_E = 1$ .

### 3.1.2 Trapezoidal rule

**Definition 3.10.** The **trapezoidal rule** is a formula based on approximating  $f(x)$  by the straight line that connects  $(a, f(a))$  and  $(b, f(b))$ .

For  $\rho(x) \equiv 1$ , it is simply

$$I_T(f) = \frac{b-a}{2} (f(a) + f(b)).$$

**Theorem 3.11.** For  $f \in C^2[a, b]$ , with weight function  $\rho \equiv 1$ , the error (remainder) of trapezoidal rule satisfies

$$\exists \xi \in [a, b], \text{ s.t. } E_T(f) = -\frac{(b-a)^3}{12} f''(\xi).$$

**Corollary 3.12.** The trapezoidal rule has  $d_E = 1$ .

### 3.1.3 Simpson's rule

**Definition 3.13.** The **Simpson's rule** is a formula based on approximating  $f(x)$  by the quadratic polynomial that goes through the points  $(a, f(a))$ ,  $(\frac{a+b}{2}, f(\frac{a+b}{2}))$  and  $(b, f(b))$ .

For  $\rho(x) \equiv 1$ , it is simply

$$I_S(f) = \frac{b-a}{6} \left( f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right).$$

**Theorem 3.14.** For  $f \in C^4[a, b]$ , with weight function  $\rho \equiv 1$ , the error (remainder) of Simpson's rule satisfies

$$\exists \xi \in [a, b], \text{ s.t. } E_S(f) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi).$$

**Corollary 3.15.** The Simpson's rule has  $d_E = 3$ .

## 3.2 Gauss Formulas

**Theorem 3.16.** For an interval  $[a, b]$  and a weight function  $\rho : [a, b] \rightarrow \mathbb{R}$ , the nodes for gauss formula  $I_n(f)$  is the root of the  $n$ th order orthogonal polynomial on  $[a, b]$  with the weight function  $\rho(x)$ .

**Theorem 3.17.** A Gauss formula  $I_n(f)$  has  $d_E = 2n - 1$ .

# Chapter 4

## Optimization

### 4.1 One-dimensional Line Search

**Definition 4.1.** Given a function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ , a initial point  $\mathbf{x}$  and a direction  $\mathbf{d}$ , denoted by  $\varphi(\alpha) = f(\mathbf{x} + \alpha\mathbf{d})$ , a **one-dimensional line search** method solves the problem

$$\varphi(\alpha) = \min_{t \in \mathbb{R}^+} \varphi(t).$$

**Method 4.2. (Success-failure method)** For a one-dimensional line search problem, the **success-failure method** is an inexact one-dimensional line search method to solve the interval  $[a, b] \in [0, +\infty)$  that exact solution  $\alpha^* \in [a, b]$ , where we

- (1) Choose initial value  $\alpha_0 \in [0, +\infty)$ ,  $h_0 > 0$ ,  $t > 0$  (commonly choose  $t = 2$ ), calculate  $\varphi(\alpha_0)$  and let  $k = 0$ ;
- (2) Let  $\alpha_{k+1} = \alpha_k + h_k$  and calculate  $\varphi(\alpha_{k+1})$ , if  $\varphi(\alpha_{k+1}) < \varphi(\alpha_k)$ , then go to (3), otherwise go to (4);
- (3) Let  $h_{k+1} = th_k$ ,  $\alpha = \alpha_k$ ,  $k = k + 1$ , and go to (2);
- (4) If  $k = 0$ , then let  $h_k = -h_k$  and go to (2), otherwise stop and the solution  $[a, b]$  satisfies  $a = \min\{\alpha, \alpha_k\}$ ,  $b = \max\{\alpha, \alpha_k\}$ .

**Definition 4.3.** A general form of one-dimensional line search method is the following three steps:

- (1) **Initialization:** given initial point  $\mathbf{x}$  and acceptable error  $\varepsilon > 0$ ,  $\delta > 0$ ;
- (2) **Iteration:** calculate the direction  $\mathbf{d}$  and step size  $\alpha$  that  $f(\mathbf{x} + \alpha\mathbf{d}) = \min_{t \in \mathbb{R}^+} f(\mathbf{x} + t\mathbf{d})$  and let  $\mathbf{x} = \mathbf{x} + \alpha\mathbf{d}$ ;
- (3) **Stop condition:** if  $\|\nabla f(\mathbf{x})\| \leq \varepsilon$  or  $U_{\mathbb{R}^n}(\mathbf{x}, \delta)$  includes the exact solution, then the current  $\mathbf{x}$  is the solution.

where the iteration step are repeated until  $\mathbf{x}$  satisfies the stop condition.

**Definition 4.4.** Given a method, denoted by  $\{\mathbf{x}_k\}$  the sequence of the iteration and  $\mathbf{x}^*$  the exact solution, the method is **(Q-)linear convergence** if

$$\lim_{k \rightarrow \infty} \frac{\|\mathbf{x}_{k+1} - \mathbf{x}^*\|}{\|\mathbf{x}_k - \mathbf{x}^*\|} \in (0, 1),$$

the method is **(Q-)sublinear convergence** if

$$\lim_{k \rightarrow \infty} \frac{\|\mathbf{x}_{k+1} - \mathbf{x}^*\|}{\|\mathbf{x}_k - \mathbf{x}^*\|} = 1,$$

the method is **(Q-)superlinear convergence** if

$$\lim_{k \rightarrow \infty} \frac{\|\mathbf{x}_{k+1} - \mathbf{x}^*\|}{\|\mathbf{x}_k - \mathbf{x}^*\|} = 0.$$

For a superlinear convergence method, the method is  $r$ -order linear convergence if

$$\lim_{k \rightarrow \infty} \frac{\|\mathbf{x}_{k+1} - \mathbf{x}^*\|}{\|\mathbf{x}_k - \mathbf{x}^*\|^r} \in [0, +\infty),$$

where when  $r = 2$  is called **(Q-)quadratic convergence**.

**Remark 4.5.** There is another **R-convergence** for judging a sequence which use another Q-convergence sequence as the boundary of  $\{\|\mathbf{x}_k - x^*\|\}$ , but is not needed here.

**Method 4.6. (Golden section method)** Given the initial point  $\mathbf{x}$ , an interval  $[a, b]$  and  $\delta > 0$ ,

- The iteration step is:
  - (1) Calculate the two testing points  $\lambda = a + (1 - k)(b - a)$  and  $\mu = a + k(b - a)$  where  $k = \frac{\sqrt{5}-1}{2}$  is the golden ratio;
  - (2) If  $\varphi(\lambda) > \varphi(\mu)$ , let  $a = \lambda$ , otherwise let  $b = \mu$ .
- The stop condition is  $b - a \leq \delta$ ;
- The solution is  $\mathbf{x} + \frac{a+b}{2}\mathbf{d}$ .

**Theorem 4.7.** The golden section method is a **linear convergent** method.

**Method 4.8. (Fibonacci method)** Given the initial point  $\mathbf{x}$ , an interval  $[a, b]$  and  $\delta > 0$ ,

- The  $k$ -th iteration step is:
  - (1) Calculate the two testing points  $\lambda = a + \frac{F_k}{F_{k+2}}(b - a)$  and  $\mu = a + \frac{F_{k+1}}{F_{k+2}}(b - a)$  where  $F_k$  is the  $k$ -th fibonacci number and  $k$ ;
  - (2) If  $\varphi(\lambda) > \varphi(\mu)$ , let  $a = \lambda$ , otherwise let  $b = \mu$ .
- The stop condition is  $b - a \leq \delta$ ;
- The solution is  $\mathbf{x} + \frac{a+b}{2}\mathbf{d}$ .

**Theorem 4.9.** The Fibonacci method is a **linear convergent** method.

**Method 4.10. (Bisection method)** Given the initial point  $\mathbf{x}$ , an interval  $[a, b]$  and  $\delta > 0$ ,

- The iteration step is:
  - (1) Calculate the midpoint  $m = \frac{a+b}{2}$  and  $\varphi(m)$ ;
  - (2) If  $\nabla f(m) \cdot \mathbf{d} < 0$ , let  $a = m$ , otherwise let  $b = m$ .
- The stop condition is  $b - a \leq \delta$ ;
- The solution is  $\mathbf{x} + \frac{a+b}{2}\mathbf{d}$ .

**Theorem 4.11.** The bisection method is a **linear convergent** method.

**Method 4.12. (Newton's method)** Given the initial point  $\mathbf{x}$  and  $\varepsilon > 0$ ,

- The iteration step is:
  - (1) Calculate  $(\nabla^2 f(\mathbf{x}))^T \cdot \mathbf{d}$  and  $(\nabla f(\mathbf{x}))^T \cdot \mathbf{d}$ ;
  - (2) Let  $\mathbf{x} = \mathbf{x} - \frac{(\nabla f(\mathbf{x}))^T \cdot \mathbf{d}}{(\nabla^2 f(\mathbf{x}))^T \cdot \mathbf{d}}$ ;
- The stop condition is  $(\nabla f(\mathbf{x}))^T \cdot \mathbf{d} \leq \varepsilon$ ;
- The solution is  $\mathbf{x}$ .

**Theorem 4.13.** The Newton's method is a **quadratic convergent** method.

## 4.2 Unconstrained Optimization

**Definition 4.14.** Given a convex function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ , a **unconstrained optimization** method solves the problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x})$$

by

- (1) **Initialization:** given initial point  $\mathbf{x}$  and acceptable error  $\varepsilon > 0$ ,  $\delta > 0$ ;
- (2) **Iteration:** calculate the direction  $\mathbf{d}$  and step size  $\alpha$ , then let  $\mathbf{x} = \mathbf{x} + \alpha\mathbf{d}$ ;
- (3) **Stop condition:** if  $\|\nabla f(\mathbf{x})\| \leq \varepsilon$  or  $U_{\mathbb{R}^n}(\mathbf{x}, \delta)$  includes the exact solution, then the current  $\mathbf{x}$  is the solution.

**Method 4.15. (Gradient descent method)** Given the initial point  $\mathbf{x}$  and  $\varepsilon > 0$ ,

- The iteration step is:
  - (1) Calculate  $\mathbf{d} = -\nabla f(\mathbf{x})$  and step size  $\alpha$  by a line search method;
  - (2) Let  $\mathbf{x} = \mathbf{x} + \alpha\mathbf{d}$ ;
- The stop condition is  $\|\nabla f(\mathbf{x})\| \leq \varepsilon$ ;
- The solution is  $\mathbf{x}$ .

**Theorem 4.16.** The gradient descent method is a **linear convergent** method.

**Method 4.17. (Quasi-Newton method)** Given the initial point  $\mathbf{x}$ ,  $\varepsilon > 0$  and a matrix  $H \in \mathbb{R}^{n \times n}$  (usually the identity matrix),

- The  $k$ -th iteration step is:
  - (1) Calculate  $\mathbf{d}_k = -H_k \nabla f(\mathbf{x}_k)$  and step size  $\alpha_k$  by a line search method;
  - (2) Let  $\mathbf{x}_k = \mathbf{x}_k + \alpha_k \mathbf{d}_k$  and  $H_{k+1} = r_k(H_k)$  where the function  $r_k$  is a **update** depends on  $\mathbf{x}_k$ ,  $\mathbf{x}_{k+1}$ ,  $\nabla f(\mathbf{x}_k)$  and  $\nabla f(\mathbf{x}_{k+1})$ ;
- The stop condition is  $\|\nabla f(\mathbf{x}_k)\| \leq \varepsilon$ ;
- The solution is  $\mathbf{x}_k$  that satisfies the stop condition.

**Definition 4.18.** Let  $\mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k$  and  $\mathbf{y}_k = \nabla f(\mathbf{x}_{k+1}) - \nabla f(\mathbf{x}_k)$ , the **Symmetric Rank-1 update (SR1)** is

$$H_{k+1} = H_k + \frac{(\mathbf{s}_k - H_k \mathbf{y}_k)(\mathbf{s}_k - H_k \mathbf{y}_k)^T}{(\mathbf{s}_k - H_k \mathbf{y}_k)^T \mathbf{y}_k}.$$

The **DFP update** is a rank-2 update defined as

$$H_{k+1} = H_k + \frac{\mathbf{s}_k \mathbf{s}_k^T}{\mathbf{s}_k^T \mathbf{y}_k} - \frac{H_k \mathbf{y}_k \mathbf{y}_k^T H_k}{\mathbf{y}_k^T H_k \mathbf{y}_k}.$$

The **BFGS update** is a rank-2 update defined as

$$H_{k+1} = H_k + \left(1 + \frac{\mathbf{y}_k^T H_k \mathbf{y}_k}{\mathbf{s}_k^T \mathbf{y}_k}\right) \frac{\mathbf{s}_k \mathbf{s}_k^T}{\mathbf{s}_k^T \mathbf{y}_k} - \frac{\mathbf{s}_k \mathbf{y}_k^T H_k + H_k \mathbf{y}_k \mathbf{s}_k^T}{\mathbf{s}_k^T \mathbf{y}_k}.$$

**Theorem 4.19.** The Quasi-Newton method is a **superlinear convergent** method.

**Method 4.20. (Newton's method)** Given the initial point  $\mathbf{x}$  and  $\varepsilon > 0$ ,

- The iteration step is:
  - (1) Calculate  $\mathbf{d} = -(\nabla^2 f(\mathbf{x}))^{-1} \nabla f(\mathbf{x})$  and step size  $\alpha$  by a line search method;
  - (2) Let  $\mathbf{x} = \mathbf{x} + \alpha\mathbf{d}$ ;
- The stop condition is  $\|\nabla f(\mathbf{x})\| \leq \varepsilon$ ;
- The solution is  $\mathbf{x}$ .

**Theorem 4.21.** The Newton's method is a **quadratic convergent** method.

# Chapter 5

## Initial Value Problem

**Definition 5.1.** For  $T \geq 0$ ,  $\mathbf{f} : \mathbb{R}^n \times [0, T] \rightarrow \mathbb{R}^n$  and  $\mathbf{u}_0 \in \mathbb{R}^n$ , the **initial value problem** (IVP) is to find  $u(t) \in C^1$  satisfies

$$\mathbf{u}' = \mathbf{f}(\mathbf{u}(t), t), \quad \mathbf{u}(0) = \mathbf{u}_0.$$

**Notation 5.2.** To numerically solve the IVP, we are given initial condition  $\mathbf{u}_0 = \mathbf{u}(t_0)$ , and want to compute approximations  $\{\mathbf{u}_k, k = 1, 2, \dots\}$  such that

$$\mathbf{u}_k \approx \mathbf{u}(t_k),$$

where  $k$  is the uniform time step size and  $t_n = nk$ .

### 5.1 Linear Multistep Method

**Definition 5.3.** For solving the IVP, an  $s$ -step **linear multistep method** (LMM) has the form

$$\sum_{j=0}^s \alpha_j \mathbf{u}_{n+j} = k \sum_{j=0}^s \beta_j \mathbf{f}(\mathbf{u}_{n+j}, t_{n+j}),$$

where  $\alpha_s = 1$  is assumed WLOG.

**Definition 5.4.** An LMM is **explicit** if  $\beta_s = 0$ , otherwise it is **implicit**.

### 5.2 Runge-Kutta Method

**Definition 5.5.** An  $s$ -stage **Runge-Kutta method** (RK) is a one-step method of the form

$$\begin{aligned} \mathbf{y}_i &= \mathbf{f} \left( \mathbf{u}_n + k \sum_{j=1}^s a_{ij} \mathbf{y}_j, t_n + c_i k \right), \\ \mathbf{u}_{i+1} &= \mathbf{u}_i + k \sum_{j=1}^s b_j \mathbf{y}_j, \end{aligned}$$

where  $i = 1, \dots, s$  and  $a_{ij}, b_j, c_i \in \mathbb{R}$ .

**Definition 5.6.** The **Butcher tableau** is one way to organize the coefficients of an RK method as follows

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

The matrix  $A = (a_{ij})_{s \times s}$  is called the RK matrix and  $\mathbf{b} = (b_1, \dots, b_s)^T$ ,  $\mathbf{c} = (c_1, \dots, c_s)^T$  are called the RK weights and the RK nodes.

**Definition 5.7.** An  $s$ -stage **collocation method** is a numerical method for solving the IVP, where we

- (1) choose  $s$  distinct collocation parameters  $c_1, \dots, c_s$ ,



- (2) seek  $s$ -degree polynomial  $p$  satisfying  
 $\forall i = 1, 2, \dots, s, \quad \mathbf{p}(t_n) = \mathbf{u}_n \quad \text{and} \quad \mathbf{p}'(t_n + c_i k) = \mathbf{f}(\mathbf{p}(t_n + c_i k), t_n + c_i k),$   
(3) set  $\mathbf{u}_{n+1} = \mathbf{p}(t_{n+1})$ .

**Theorem 5.8.** The  $s$ -stage collocation method is an  $s$ -stage IRK method with

$$a_{ij} = \int_0^{c_i} l_j(\tau) d\tau, \quad b_j = \int_0^1 l_j(\tau) d\tau,$$

where  $i, j = 1, \dots, s$  and  $l_k(\tau)$  is the elementary Lagrange interpolation polynomial.

## 5.3 Theoretical analysis

**Definition 5.9.** A function  $\mathbf{f} : \mathbb{R}^n \times [0, +\infty) \rightarrow \mathbb{R}^n$  is **Lipschitz continuous** in its first variable over some domain

$$\Omega = \{(\mathbf{u}, t) : \|\mathbf{u} - \mathbf{u}_0\| \leq a, t \in [0, T]\}$$

iff

$$\exists L \geq 0, \quad \text{s.t. } \forall (\mathbf{u}, t) \in \Omega, \quad \|\mathbf{f}(\mathbf{u}, t) - \mathbf{f}(\mathbf{v}, t)\| \leq L \|\mathbf{u} - \mathbf{v}\|.$$

### 5.3.1 Error analysis

**Definition 5.10.** The **local truncation error**  $\tau$  is the error caused by replacing continuous derivatives with numerical formulas.

**Definition 5.11.** A numerical formulas is **consistent** if  $\lim_{k \rightarrow 0} \tau = 0$ .

### 5.3.2 Stability

**Definition 5.12.** The **region of absolute stability** (RAS) of a numerical method, applied to

$$\mathbf{u}' = \lambda \mathbf{u}, \quad \mathbf{u}_0 = \mathbf{u}(t_0),$$

is the region  $\Omega$  that

$$\forall \mathbf{u}_0, \quad \forall \lambda k \in \Omega, \quad \lim_{n \rightarrow +\infty} \mathbf{u}_n = 0.$$

**Definition 5.13.** The **stability function** of a one-step method is a function  $R : \mathbb{C} \rightarrow \mathbb{C}$  that satisfies

$$\mathbf{u}_{n+1} = R(z) \mathbf{u}_n$$

for the  $\mathbf{u}' = \lambda \mathbf{u}$  where  $\text{Re}(E(\lambda)) \leq 0$  and  $z = k\lambda$ .

**Definition 5.14.** A numerical method is **stable** or **zero stable** iff its application to any IVP with  $\mathbf{f}(\mathbf{u}, t)$  Lipschitz continuous in  $\mathbf{u}$  and continuous in  $t$  yields

$$\forall T > 0, \quad \lim_{k \rightarrow 0, Nk=T} \|\mathbf{u}_N\| < \infty.$$

**Definition 5.15.** A numerical method is **A( $\alpha$ )-statble** if the region of absolute stability  $\Omega$  satisfies

$$\{z \in \mathbb{C} : \pi - \alpha \leq \arg(z) \leq \pi + \alpha\} \subseteq \Omega.$$

**Definition 5.16.** A numerical method is **A-statble** if the region of absolute stability  $\Omega$  satisfies

$$\{z \in \mathbb{C} : \text{Re}(z) \leq 0\} \subseteq \Omega.$$

**Definition 5.17.** A one-step method is **L-stable** if it is A-stable, and its stability function satisfies

$$\lim_{z \rightarrow \infty} |R(z)| = 0.$$

**Definition 5.18.** An one-step method is **I-stable** iff its stability function satisfies

$$\forall y \in \mathbb{R}, |R(yi)| \leq 1.$$

**Definition 5.19.** An one-step method is **B-stable** (or **contractive**) if for any contractive ODE system, every pair of its numerical solutions  $\mathbf{u}_n$  and  $\mathbf{v}_n$  satisfy

$$\forall n \in \mathbb{N}, \|u_{n+1} - v_{n+1}\| \leq \|u_n - v_n\|.$$

**Definition 5.20.** An RK method is **algebraically stable** iff the RK weights  $b_1, \dots, b_s$  are nonnegative, the **algebraic stability matrix**  $M = (b_i a_{ij} + b_i a_{ji} - b_i b_j)_{s \times s}$  is positive semidefinite.

**Theorem 5.21.** The order of accuracy of an implicit A-stable LMM satisfies  $p \leq 2$ . An explicit LMM cannot be A-stable.

**Theorem 5.22.** No ERK method is A-stable.

**Theorem 5.23.** An RK method is A-stable if and only if it is I-stable and all poles of its stability function  $R(z)$  have positive real parts.

**Theorem 5.24.** If an A-stable RK method with a nonsingular RK matrix  $A$  is stiffly accurate, then it is L-stable.

**Theorem 5.25.** If an A-stable RK method with a nonsingular RK matrix  $A$  satisfies

$$\forall i \in \{1, \dots, s\}, \quad a_{i1} = b_i,$$

then it is L-stable.

**Theorem 5.26.** B-stable one-step methods are A-stable.

**Theorem 5.27.** An algebraically stable RK method is B-stable and A-stable.

### 5.3.3 Convergence

**Definition 5.28.** A numerical method is convergent iff its application to any IVP with  $\mathbf{f}(\mathbf{u}, t)$  Lipschitz continuous in  $\mathbf{u}$  and continuous in  $t$  yields

$$\forall T > 0, \quad \lim_{k \rightarrow 0, nk=T} \mathbf{u}_n = \mathbf{u}(T).$$

**Theorem 5.29.** A numerical method is convergent iff it is consistent and stable.

## 5.4 Important Methods

### 5.4.1 Forward Euler's method

**Definition 5.30.** The **forward Euler's method** solves the IVP by

$$\mathbf{u}_{n+1} = \mathbf{u}_n + k\mathbf{f}(\mathbf{u}_n, t_n).$$

**Theorem 5.31.** The region of absolute stability for forward Euler's method is

$$\{z \in \mathbb{C} : |1 + z| \leq 1\}.$$

### 5.4.2 Backward Euler's method

**Definition 5.32.** The **backward Euler's method** solves the IVP by

$$\mathbf{u}_{n+1} = \mathbf{u}_n + k\mathbf{f}(\mathbf{u}_{n+1}, t_{n+1}).$$

**Theorem 5.33.** The region of absolute stability for backward Euler's method is

$$\{z \in \mathbb{C} : |1 - z| \geq 1\}.$$

### 5.4.3 Trapezoidal method

**Definition 5.34.** The **trapezoidal method** solves the IVP by

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \frac{k}{2}(\mathbf{f}(\mathbf{u}_n, t_n) + \mathbf{f}(\mathbf{u}_{n+1}, t_{n+1})).$$

**Theorem 5.35.** The region of absolute stability for trapezoidal method is

$$\left\{ z \in \mathbb{C} : \left| \frac{2+z}{2-z} \right| \geq 1 \right\}.$$

### 5.4.4 Midpoint method (Leapfrog method)

**Definition 5.36.** The **midpoint method (Leapfrog method)** solves the IVP by

$$\mathbf{u}_{n+1} = \mathbf{u}_{n-1} + 2k\mathbf{f}(\mathbf{u}_n, t_n).$$

**Theorem 5.37.** The region of absolute stability for midpoint method is

$$\left\{ z \in \mathbb{C} : \left| z \pm \sqrt{1+z^2} \right| \leq 1 \right\} \stackrel{?}{=} \{0\}.$$

### 5.4.5 Heun's third-order RK method

**Definition 5.38.** The **Heun's third-order formula** is an ERK method of the form

$$\begin{cases} \mathbf{y}_1 &= \mathbf{f}(\mathbf{u}_n, t_n), & 0 & \left| \begin{array}{ccc} 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{2}{3} & 0 & \frac{2}{3} & 0 \end{array} \right. \\ \mathbf{y}_2 &= \mathbf{f}\left(\mathbf{u}_n + \frac{k}{3}\mathbf{y}_1, t_n + \frac{k}{3}\right), & \frac{1}{3} & \\ \mathbf{y}_3 &= \mathbf{f}\left(\mathbf{u}_n + \frac{2k}{3}\mathbf{y}_2, t_n + \frac{2k}{3}\right), & \frac{2}{3} & \\ \mathbf{u}_{n+1} &= \mathbf{u}_n + \frac{k}{4}(\mathbf{y}_1 + 3\mathbf{y}_3). & \frac{1}{4} & \left| \begin{array}{ccc} 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{2}{3} & 0 & \frac{2}{3} & 0 \end{array} \right. \end{cases}$$

### 5.4.6 Classical fourth-order RK method

**Definition 5.39.** The **classical fourth-order RK method** is an ERK method of the form

$$\begin{cases}
\mathbf{y}_1 &= \mathbf{f}(\mathbf{u}_n, t_n), & 0 & \left| \begin{array}{cccc} 0 & 0 & 0 & 0 \end{array} \right. \\
\mathbf{y}_2 &= \mathbf{f}\left(\mathbf{u}_n + \frac{k}{2}\mathbf{y}_1, t_n + \frac{k}{2}\right), & \frac{1}{2} & \left| \begin{array}{cccc} \frac{1}{2} & 0 & 0 & 0 \end{array} \right. \\
\mathbf{y}_3 &= \mathbf{f}\left(\mathbf{u}_n + \frac{k}{2}\mathbf{y}_2, t_n + \frac{k}{2}\right), & \frac{1}{2} & \left| \begin{array}{cccc} 0 & \frac{1}{2} & 0 & 0 \end{array} \right. \\
\mathbf{y}_4 &= \mathbf{f}(\mathbf{u}_n + k\mathbf{y}_3, t_n + k), & 1 & \left| \begin{array}{cccc} 0 & 0 & 1 & 0 \end{array} \right. \\
\mathbf{u}_{n+1} &= \mathbf{u}_n + \frac{k}{6}(\mathbf{y}_1 + 2\mathbf{y}_2 + 2\mathbf{y}_3 + \mathbf{y}_4). & \hline & \left| \begin{array}{cccc} \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \right.
\end{cases}$$

### 5.4.7 TR-BDF2 method

**Definition 5.40.** The **TR-BDF2 method** is an one-step method of the form

$$\begin{cases}
\mathbf{u}_* &= \mathbf{u}_n + \frac{k}{4}(\mathbf{f}(\mathbf{u}_n, t_n) + \mathbf{f}(\mathbf{u}_*, t_n + \frac{k}{2})), \\
\mathbf{u}_{n+1} &= \frac{1}{3}(4\mathbf{u}_* - \mathbf{u}_n + k\mathbf{f}(\mathbf{u}_{n+1}, t_{n+1})).
\end{cases}$$

# Chapter 6

## Number Theory

### 6.1 Prime Number

**Definition 6.1.** A **prime number** (or a **prime**) is a natural number greater than 1 that is not a product of two smaller natural numbers.

**Definition 6.2.** A **composite number** (or a **composite**) is a natural number greater than 1 that is a product of two smaller natural numbers.

#### 6.1.1 Primality testing

**Theorem 6.3.** For a integer  $n \in \mathbb{N}$ , if it is a product of two natural number  $a$  and  $b$  thar  $a \leq b$ , then

$$1 \leq a \leq \sqrt{n} \leq b \leq n.$$

**Method 6.4. (Trial division)** Given a integer  $n$ , the **trial division method** divides  $n$  by each integer from 2 up to  $\sqrt{n}$ . Any such integer dividing  $n$  evenly establishes  $n$  as composite, otherwise it is prime.

**Theorem 6.5. (Fermat's little theorem)** For a prime number  $p$  and a number  $a$  that  $\gcd(a, p) = 1$ , then  $a^{p-1} \equiv 1 \pmod{p}$

**Method 6.6.** The **Miller-Rabin** algorithm is a method of primality testing, where given a number  $n$ , where we

- (1) determine directly for small numbers such as  $p = 2$ .
- (2) factorize the number  $p = u \times 2^t$ ;
- (3) choose a number  $a$  that  $\gcd(a, p) = 1$ , and calculate  $a^u, a^{u \times 2}, a^{u \times 2^2}, \dots, a^{u \times 2^{t-1}}$ ;
- (4) if  $a^u \equiv 1 \pmod{p}$ , or  $\exists a^{u \times k}, k < t$  that  $a^{u \times k} \equiv p - 1 \pmod{p}$  then  $p$  passes the test, otherwise,  $p$  is a composite number;
- (5) repeat above steps to eliminate error.

For numbers less than  $2^{32}$ , choose  $a \in \{2, 7, 61\}$  is enough, for numbers less than  $2^{64}$ , choose  $a \in \{2, 325, 9375, 28178, 450775, 9780504, 1795265022\}$  is enough.

#### 6.1.2 Sieves

**Method 6.7. (Sieve of Eratosthenes)** Given a upper limit  $n$ , the **sieve of Eratosthenes** solves all the prime numbers up to  $n$  by marking composite numbers, where we

- (1) create a list of consecutive integers from 2 to  $n$ :  $\{2, 3, 4, \dots, n\}$ ;
- (2) initially, let  $p = 2$ , the smallest prime number;
- (3) enumerate the multiples of  $p$  by counting in increments of  $p$  from  $2p$  to  $n$ , and mark them in the list;
- (4) find the smallest number in the list greater than  $p$  that is not marked;
- (5) if there was no such number, the method is terminated and the numbers remaining not marked in the list are all the primes below  $n$ , otherwise let  $p$  now equal the new number which is the next prime, and repeat from step (3).