

Handbook of Applied Mathematics

Zeyu Wang¹

May 12, 2024

¹Email: zeyuwang@zuua.zju.edu.cn

Contents

Contents	i
Mathematical Foundation	1
1 Analysis	2
1.1 Calculus	2
1.1.1 Gauss-Green Theorem (Divergence Theorem)	2
1.2 Important Inequalities	2
1.2.1 Fundamental inequality	2
1.2.2 Triangle inequality	2
1.2.3 Bernoulli inequality	2
1.2.4 Jensen's inequality	2
1.2.5 Cauchy-Schwarz inequality	3
1.2.6 Hölder's inequality	3
1.2.7 Young's inequality	3
1.2.8 Minkowski inequality	4
1.3 Special Functions	4
1.3.1 Gaussian function	4
1.3.2 Dirac delta function	4
1.3.3 Gamma function	4
1.3.4 Beta Function	5
2 Algebra	6
2.1 Linear Space	6
2.1.1 Linear map	6
2.2 Metric Space	7
2.2.1 Completeness & Compactness	8
2.2.2 Cover	8
2.2.3 Cantor's intersection Theorem	8
2.2.4 Cluster point	8
2.3 Normed Space	9
2.4 Inner Product Space	9
2.4.1 Orthonormal system	9
2.5 Banach Space	10
2.6 Hilbert Space	10
2.7 Single Variable Polynomial	10
2.8 Orthogonal Polynomial	11
2.8.1 Legendre polynomial	11
2.8.2 Chebyshev polynomial of the first kind	11
2.8.3 Chebyshev polynomial of the second kind	12
2.8.4 Laguerre polynomial	12
2.8.5 Hermite polynomial (probability theory form)	12

3	Probability Theory	14
3.1	Discrete random variables	14
3.2	Continuous random variables	14
3.3	Characteristic functions	14
3.4	Probability limit theorems	14
4	Stochastic Process	15
4.1	Poisson process	15
4.2	Markov chain	15
5	Statistics	16
6	Graph	17
6.1	Shortest Path	17
6.2	Matching	17
6.3	Network Flow	17
6.4	Tree	17
7	Combinatorics	18
7.1	Generating function	18
7.2	Inclusion–exclusion principle	18
7.3	Special Numbers	18
7.3.1	Catalan number	18
7.3.2	Stirling number	18
	Scientific Computing	19
8	Interpolation	20
8.1	Polynomial Interpolation	20
8.1.1	Lagrange formula	20
8.1.2	Newton formula	20
8.1.3	Neville-Aitken algorithm	20
8.1.4	Hermite interpolation	21
8.1.5	Approximation	21
8.1.6	Error analysis	22
8.2	Spline	22
8.2.1	Cubic spline	22
8.2.2	B-spline	23
8.2.3	Error analysis	23
9	Integration	24
9.1	Newton-Cotes Formulas	24
9.1.1	Midpoint rule	24
9.1.2	Trapezoidal rule	25
9.1.3	Simpson’s rule	25
9.2	Gauss Formulas	25
10	Optimization	26
10.1	One-dimensional Line Search	26
10.2	Unconstrained Optimization	27
11	Initial Value Problem	29
11.1	Linear Multistep Method	29

11.2	Runge-Kutta Method	29
11.3	Theoretical analysis	30
11.3.1	Error analysis	30
11.3.2	Stability	30
11.3.3	Convergence	31
11.4	Important Methods	31
11.4.1	Forward Euler's method	32
11.4.2	Backward Euler's method	32
11.4.3	Trapezoidal method	32
11.4.4	Midpoint method (Leapfrog method)	32
11.4.5	Heun's third-order RK method	32
11.4.6	Classical fourth-order RK method	32
11.4.7	TR-BDF2 method	33
12	Number Theory	34
12.1	Prime Number	34
12.1.1	Primality testing	34
12.1.2	Sieves	34
	Machine Learning	35
13	Regression	36
13.1	Linear Regression	36
14	Decision Tree	37
15	Support Vector Machine	38
16	Cluster	39
17	Neural Networks	40

Part 1

Mathematical Foundation

Chapter 1

Analysis

1.1 Calculus

1.1.1 Gauss-Green Theorem (Divergence Theorem)

Theorem 1.1. (Gauss-Green Theorem (Divergence Theorem)) For a bounded open set $\Omega \in \mathbb{R}^n$ that $\partial\Omega \in C^1$ and a function $\mathbf{F}(\mathbf{x}) = (F_1(\mathbf{x}), \dots, F_n(\mathbf{x})) : \overline{\Omega} \rightarrow \mathbb{R}^n$ satisfies $\mathbf{F}(\mathbf{x}) \in C^1(\Omega) \cap C(\overline{\Omega})$,

$$\int_{\Omega} \operatorname{div} \mathbf{F}(\mathbf{x}) d\mathbf{x} = \int_{\partial\Omega} \mathbf{F}(\mathbf{x}) \cdot \mathbf{n} dS(x),$$

where \mathbf{n} is outward pointing unit normal vector at $\partial\Omega$.

1.2 Important Inequalities

1.2.1 Fundamental inequality

Theorem 1.2. (Fundamental inequality)

$$\forall x, y \in \mathbb{R}^+, \frac{2}{\frac{1}{a} + \frac{1}{b}} \leq \sqrt{ab} \leq \frac{a+b}{2} \leq \sqrt{\frac{a^2 + b^2}{2}}, \text{ equality holds iff } a = b.$$

1.2.2 Triangle inequality

Theorem 1.3. (Triangle inequality)

$$\begin{aligned} a, b \in \mathbb{C}, \quad ||a| - |b|| \leq |a \pm b| \leq |a| + |b|, \\ \mathbf{a}, \mathbf{b} \in \mathbb{R}^n, \quad ||\mathbf{a}| - |\mathbf{b}|| \leq \|\mathbf{a} \pm \mathbf{b}\| \leq \|\mathbf{a}\| + \|\mathbf{b}\|. \end{aligned}$$

1.2.3 Bernoulli inequality

Theorem 1.4. (Bernoulli inequality)

$$\begin{aligned} \forall x \in (-1, +\infty), \forall a \in [1, +\infty), \quad (1+x)^a &\geq 1+ax, \\ \forall x \in (-1, +\infty), \forall a \in (0, 1), \quad (1+x)^a &\leq 1+ax, \\ \forall x \in (-1, +\infty), \forall a \in (-1, 0), \quad (1+x)^a &\geq 1+ax, \\ \forall x_i \in \mathbb{R}, i \in \{1, \dots, n\}, \quad \prod_{i=1}^n (1+x_i) &\geq 1 + \sum_{i=1}^n x_i, \\ \forall y \geq x > 0, \quad (1+x)^y &\geq (1+y)^x. \end{aligned}$$

1.2.4 Jensen's inequality

Theorem 1.5. (Jensen's inequality) For a real convex function $f(x) : [a, b] \rightarrow \mathbb{R}$, numbers $x_1, \dots, x_n \in [a, b]$ and weights a_1, \dots, a_n , the Jensen's inequality can be start as

$$\frac{\sum_{i=1}^n a_i f(x_i)}{\sum_{i=1}^n a_i} \geq f\left(\frac{\sum_{i=1}^n a_i x_i}{\sum_{i=1}^n a_i}\right).$$

And for concave function f ,

$$\frac{\sum_{i=1}^n a_i f(x_i)}{\sum_{i=1}^n a_i} \leq f\left(\frac{\sum_{i=1}^n a_i x_i}{\sum_{i=1}^n a_i}\right).$$

Equality holds iff $x_1 = \dots = x_n$ or f is linear on $[a, b]$.

1.2.5 Cauchy–Schwarz inequality

Theorem 1.6. (Cauchy–Schwarz inequality)

Discrete form. For real numbers $a_1, \dots, a_n, b_1, \dots, b_n \in \mathbb{R}, n \geq 2$

$$\sum_{i=1}^n a_i^2 \sum_{i=1}^n b_i^2 \geq \left(\sum_{i=1}^n a_i b_i \right)^2.$$

Equality holds iff $\frac{a_1}{b_1} = \dots = \frac{a_n}{b_n}$ or $a_i = 0$ or $b_i = 0$.

Inner product form. For a inner product space V with a norm induced by the inner product,

$$\forall \mathbf{a}, \mathbf{b} \in V \quad \|\mathbf{a}\| \cdot \|\mathbf{b}\| \geq |\langle \mathbf{a}, \mathbf{b} \rangle|.$$

Equality holds iff $\exists k \in \mathbb{R}$, s.t. $k\mathbf{a} = \mathbf{b}$ or $\mathbf{a} = k\mathbf{b}$.

Probability form. For random variables X and Y ,

$$\sqrt{E(X^2)} \cdot \sqrt{E(Y^2)} \geq |E(XY)|.$$

Equality holds iff $\exists k \in \mathbb{R}$, s.t. $kX = Y$ or $X = kY$.

Integral form. For integrable functions $f, g \in L^2(\Omega)$,

$$\int_{\Omega} f^2(x) dx + \int_{\Omega} g^2(x) dx \geq \left(\int_{\Omega} f(x)g(x) dx \right)^2.$$

Equality holds iff $\exists k \in \mathbb{R}$, s.t. $kf(x) = g(x)$ or $f(x) = kg(x)$.

1.2.6 Hölder's inequality

Theorem 1.7. (Hölder's inequality)

Discrete form. For real numbers $a_1, \dots, a_n, b_1, \dots, b_n \in \mathbb{R}, n \geq 2$ and $p, q \in [1, +\infty)$ that $\left(\frac{1}{p}\right) + \left(\frac{1}{q}\right) = 1$,

$$\left(\sum_{i=1}^n a_i^p \right)^{\frac{1}{p}} \left(\sum_{i=1}^n b_i^q \right)^{\frac{1}{q}} \geq \left(\sum_{i=1}^n a_i b_i \right).$$

Equality holds iff $\exists c_1, c_2 \in \mathbb{R}, c_1^2 + c_2^2 \neq 0$, s.t. $c_1 a_i^p = c_2 b_i^q$.

Integral form. For functions $f \in L^p(\Omega), g \in L^q(\Omega)$ and $p, q \in [1, +\infty)$ that $\left(\frac{1}{p}\right) + \left(\frac{1}{q}\right) = 1$,

$$\left(\int_{\Omega} |f(x)|^p dx \right)^{\frac{1}{p}} + \left(\int_{\Omega} |g(x)|^q dx \right)^{\frac{1}{q}} \geq \int_{\Omega} f(x)g(x) dx.$$

1.2.7 Young's inequality

Theorem 1.8. (Young's inequality) For $p, q \in [1, +\infty)$ that $\frac{1}{p} + \frac{1}{q} = 1$,

$$\forall a, b \in \mathbb{R}^*, \frac{a^p}{p} + \frac{b^q}{q} \geq ab.$$

Equality holds iff $a^p = b^q$.

1.2.8 Minkowski inequality

Theorem 1.9. (Minkowski inequality) For a metric space S ,

$$\forall f, g \in L^p(S), p \in [1, +\infty], \|f\|_p + \|g\|_p \geq \|f + g\|_p.$$

For $p \in (1, +\infty)$, equality holds iff $\exists k \geq 0$, s.t. $f = kg$ or $kf = g$.

1.3 Special Functions

1.3.1 Gaussian function

Definition 1.10. A **Gaussian function**, or a **Gaussian**, is a function of the form

$$f(x) = a \exp\left(-\frac{(x-b)^2}{2c^2}\right),$$

where $a \in \mathbb{R}^+$ is the height of the curve's peak, $b \in \mathbb{R}$ is the position of the center of the peak and $c \in \mathbb{R}^+$ is the standard deviation or the Gaussian root mean square width.

Theorem 1.11. The integral of a Gaussian is

$$\int_{-\infty}^{+\infty} a \exp\left(-\frac{(x-b)^2}{2c^2}\right) dx = ac\sqrt{2\pi}.$$

Definition 1.12. A **normal distribution** or a **Gaussian distribution** is a continuous probability distribution of the form

$$f_{\mu,\sigma}(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right),$$

where μ is the mean and σ is the standard deviation.

1.3.2 Dirac delta function

Definition 1.13. The **Dirac delta function** centered at \bar{x} is

$$\delta(x - \bar{x}) = \lim_{\varepsilon \rightarrow 0} f_{\bar{x},\varepsilon}(x - \bar{x}),$$

where $f_{\bar{x},\varepsilon}$ is a normal distribution with its mean at \bar{x} and its standard deviation as ε .

Theorem 1.14. The Dirac delta function satisfies

$$\delta(x - \bar{x}) = \begin{cases} +\infty, & x = \bar{x} \\ 0, & x \neq \bar{x} \end{cases} \quad \int_{-\infty}^x \delta(x - \bar{x}) dx = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0 \end{cases}$$

where $H(x) = \int_{-\infty}^x \delta(x - \bar{x}) dx$ is called **Heaviside function** or **step function**.

Theorem 1.15. If $f : \mathbb{R} \rightarrow \mathbb{R}$ is continuous, then

$$\int_{-\infty}^{+\infty} \delta(x - \bar{x}) f(x) dx = f(\bar{x}).$$

1.3.3 Gamma function

Definition 1.16. The **Gamma function** defined on \mathbb{C} is

$$\Gamma(z) = \int_0^{+\infty} t^{z-1} e^{-t} dt,$$

where $\text{Re}(z) > 0$.

Theorem 1.17. The Gamma function satisfies

$$\begin{aligned}\forall x \in \mathbb{C}, \quad \Gamma(x+1) &= x\Gamma(x), \\ \forall n \in \mathbb{N}^*, \Gamma(n) &= (n-1)!. \end{aligned}$$

Theorem 1.18. The Gamma function satisfies

$$\forall x \in (0, 1), \Gamma(1-x)\Gamma(x) = \frac{\pi}{\sin(\pi x)},$$

which implies

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}.$$

1.3.4 Beta Function

Definition 1.19. For $p, q \in \mathbb{R}^+$, the **Beta function** is defined as

$$B(p, q) = \int_0^1 x^{p-1}(1-x)^{q-1} dx.$$

Theorem 1.20. The Beta function satisfies

$$\forall p, q \in \mathbb{R}^+, B(p, q) = B(q, p) = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}.$$

Theorem 1.21. The Beta function satisfies

$$\begin{aligned}\forall p > 0, \forall q > 1, B(p, q) &= \frac{q-1}{p+q-1} B(p, q-1), \\ \forall p > 1, \forall q > 0, B(p, q) &= \frac{p-1}{p+q-1} B(p-1, q), \\ \forall p > 1, \forall q > 1, B(p, q) &= \frac{(p-1)(q-1)}{(p+q-1)(p+q-2)} B(p-1, q-1). \end{aligned}$$

Chapter 2

Algebra

2.1 Linear Space

Definition 2.1. (Linear Space) A linear space over a field \mathbb{F} is a nonempty set V with a addition and a scalar multiplication that satisfies

- (1) Associativity of addition: $\forall \mathbf{x}, \mathbf{y} \in V, \mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$,
- (2) Commutativity of addition: $\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in V, (\mathbf{x} + \mathbf{y}) + \mathbf{z} = \mathbf{x} + (\mathbf{y} + \mathbf{z})$,
- (3) Identity element of addition: $\exists \mathbf{0} \in V, \forall \mathbf{x}, \mathbf{x} + \mathbf{0} = \mathbf{x}$,
- (4) Inverse elements of addition: $\forall \mathbf{x} \in V, \exists \mathbf{y} \in V, \text{ s.t. } \mathbf{x} + \mathbf{y} = \mathbf{0}$,
- (5) Compatibility of multiplication: $\forall \mathbf{x} \in V, a, b \in \mathbb{F}, (ab)\mathbf{x} = a(b\mathbf{x})$,
- (6) Identity element of multiplication: $\exists 1 \in \mathbb{F}, \forall \mathbf{x} \in V, 1\mathbf{x} = \mathbf{x}$,
- (7) Distributivity: $\forall \mathbf{x} \in V, a, b \in \mathbb{F}, (a + b)\mathbf{x} = a\mathbf{x} + b\mathbf{x}$,
- (8) Distributivity: $\forall \mathbf{x}, \mathbf{y} \in V, a \in \mathbb{F}, a(\mathbf{x} + \mathbf{y}) = a\mathbf{x} + a\mathbf{y}$.

Notation 2.2. The **dimension** of a linear space V is written as $\dim(V)$.

Definition 2.3. Denoted by V_1, \dots, V_n linear spaces over a field \mathbb{F} , the **product of linear spaces** is defined as

$$V_1 \times \dots \times V_n = \{(\mathbf{v}_1, \dots, \mathbf{v}_n) : \mathbf{v}_1 \in V_1, \dots, \mathbf{v}_n \in V_n\},$$

which is also a linear space over \mathbb{F} .

Definition 2.4. Given a linear space V , a subspace $U \subset V$ and $\mathbf{v} \in V$, the **coset** (or **affine subset**) is defined as

$$\bar{\mathbf{v}} = \{\mathbf{w} \in V : \mathbf{w} = \mathbf{v} + \mathbf{u}, \mathbf{u} \in U\}.$$

Definition 2.5. Given a linear space V and a subspace $U \subset V$, the **quotient space** is defined as

$$V/U = \{\mathbf{v} + U : \mathbf{v} \in V\}.$$

2.1.1 Linear map

Definition 2.6. Denoted by V and W the linear spaces over a field \mathbb{F} , a function $f : V \rightarrow W$ is called a linear map between V and W if it satisfies

- (1) Additivity: $\forall \mathbf{x}, \mathbf{y} \in V, f(\mathbf{x} + \mathbf{y}) = f(\mathbf{x}) + f(\mathbf{y})$;
- (2) Homogeneity: $\forall \mathbf{x} \in V, \forall k \in \mathbb{F}, f(k\mathbf{x}) = kf(\mathbf{x})$.

Notation 2.7. Denoted by $\mathcal{L}(V, W)$ the set of all linear maps between V and W (it also be written as $\mathcal{L}(V)$ if $V = W$).

Theorem 2.8. For linear space V, W over a field \mathbb{F} and linear maps $f, g \in \mathcal{L}(V, W)$, if we define

$$\forall \mathbf{x} \in V, \forall k \in \mathbb{F}, (f + g)(\mathbf{x}) = f(\mathbf{x}) + g(\mathbf{x}) \text{ and } (kf)(\mathbf{x}) = kf(\mathbf{x}),$$

then $\mathcal{L}(V, W)$ is a linear space.

Theorem 2.9. For a linear map $f \in \mathcal{L}(V, W)$, $f(\mathbf{0}) = f(0\mathbf{v}) = 0f(\mathbf{v}) = \mathbf{0}$.

Theorem 2.10. Given $\mathbf{v}_1, \dots, \mathbf{v}_n$ the basis of linear space V and $\mathbf{w}_1, \dots, \mathbf{w}_n$ the basis of linear space W , then there exists the only linear map $f \in \mathcal{L}(V, W)$ such that

$$\forall i \in \{1, \dots, n\}, f(\mathbf{v}_i) = \mathbf{w}_i.$$

Definition 2.11. For a linear map $f \in \mathcal{L}(V, W)$, the **kernal** (or **null space**) of f is defined as

$$\ker(f) = \{\mathbf{v} \in V : f(\mathbf{v}) = \mathbf{0}\},$$

where $\ker(f)$ is a subspace of V and the number $\dim(\ker(f))$ is the **nullity** of f which also written as $\text{nullity}(f)$

Definition 2.12. For a linear map $f \in \mathcal{L}(V, W)$, the **image** of f is defined as

$$\text{im}(f) = \{\mathbf{w} \in W : \mathbf{w} = f(\mathbf{v}), \mathbf{v} \in V\},$$

where $\text{im}(f)$ is a subspace of W and the number $\dim(\text{im}(f))$ is the **dimension** (or **rank**) of f which also written as $\text{rank}(f)$

Theorem 2.13. (Rank–nullity theorem) For a linear map $f \in \mathcal{L}(V, W)$,

$$\dim(\ker(f)) + \dim(\text{im}(f)) = \dim(V).$$

Definition 2.14. A **isomorphism** is a invertible linear map.

Definition 2.15. Two linear spaces are called **isomorphic** if there exists a invertible linear map between them.

Theorem 2.16. Two linear spaces V, W over a field \mathbb{F} are isomorphic iff $\dim(V) = \dim(W)$.

Theorem 2.17. For a linear space V that $\dim(V) < +\infty$ and a linear map $f \in \mathcal{L}(V)$, the following statements are equivalent:

- (1) f is invertible;
- (2) f is injective;
- (3) f is surjective.

2.2 Metric Space

Definition 2.18. (Metric) For a nonempty set X , the **metric** is a function $d : X \times X \rightarrow \mathbb{R}$ that satisfies

- (1) Positive definiteness: $\forall \mathbf{x}, \mathbf{y} \in X, d(\mathbf{x}, \mathbf{y}) \geq 0, d(\mathbf{x}, \mathbf{y}) \Leftrightarrow \mathbf{x} = \mathbf{y}$,
- (2) Symmetry: $\forall \mathbf{x}, \mathbf{y} \in X, d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x})$,
- (3) Triangle inequality: $\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in V, d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z}) \geq d(\mathbf{x}, \mathbf{z})$,

Definition 2.19. (Metric space) A **metric space** is a set X provided with a metric.

Notation 2.20. (Neighbourhood) For a metric space X , the **neighbourhood** of $\mathbf{x} \in X$ with radius $\varepsilon > 0$ is defined as

$$U_X(\mathbf{x}, \varepsilon) = \{t : d(\mathbf{x}, t) < \varepsilon, t \in X\}.$$

Notation 2.21. (Punctured neighbourhood) For a metric space X , the **punctured neighbourhood** of $\mathbf{x} \in X$ with radius $\varepsilon > 0$ is defined as

$$U_X^\circ(\mathbf{x}, \varepsilon) = U_X(\mathbf{x}, \varepsilon) \setminus \{\mathbf{x}\} = \{t : d(\mathbf{x}, t) < \varepsilon, t \in X \setminus \{\mathbf{x}\}\}.$$

2.2.1 Completeness & Compactness

Theorem 2.22. (Cauchy's convergence test) A sequence $\{\mathbf{x}_n\}$ in a metric space X is convergent (or said a **cauchy sequence**) iff

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}, \text{ s.t. } \forall m, n > N, \|\mathbf{x}_n - \mathbf{x}_m\| < \varepsilon.$$

Definition 2.23. (Completeness) A metric space X is **complete** iff all cauchy sequence of X is convergent in X .

Theorem 2.24. (Supremum and infimum principle) For a nonempty set X , if the upper/lower bound of X exists, then the supremum/infimum of X exists.

Theorem 2.25. (The monotone bounded convergence Theorem) For a bounded sequence $\{\mathbf{x}_n\}$, if it is increased, then

$$\lim_{n \rightarrow \infty} \mathbf{x}_n = \sup\{\mathbf{x}_n : n \in \mathbb{N}\}.$$

If it is decreased, then

$$\lim_{n \rightarrow \infty} \mathbf{x}_n = \inf\{\mathbf{x}_n : n \in \mathbb{N}\}.$$

2.2.2 Cover

Definition 2.26. (Cover) For a metric space $S \subseteq X$, A **cover** of S is a set of open sets $\{D_n\}$ satisfies

$$\forall \mathbf{x} \in X, \exists D_n, \text{ s.t. } \mathbf{x} \in D_n.$$

Definition 2.27. (Compactness) A metric space X is called **compact** if every open cover of X has a finite subcover.

2.2.3 Cantor's intersection Theorem

Theorem 2.28. (Cantor's intersection Theorem) For a decreasing sequence of nested non-empty compact, closed subsets $S_n \subseteq X, n \in \mathbb{N}$ of a metric space, if $\{S_n\}$ satisfies

$$S_0 \supset S_1, \dots, \supset S_n \supset \dots,$$

then

$$\bigcap_{k=0}^{\infty} S_k \neq \emptyset.$$

where there is only one point $\mathbf{x} \in \bigcap_{k=0}^{\infty} S_k$ for a complete metric space.

Corollary 2.29. For decreasing sequence of nested non-empty compact, closed subsets $S_n \in X, n \in \mathbb{N}$ of a complete metric space and $\{\mathbf{x}\} = \bigcap_{k=0}^{\infty} S_k$, then

$$\forall \varepsilon > 0, \exists N > 0, \text{ s.t. } \forall n > N, X_n \subset U_X(x, \varepsilon).$$

2.2.4 Cluster point

Definition 2.30. (Cluster point) For a metric space $S \subseteq X$, the **cluster point** of S is the point $\mathbf{x} \in X$ satisfies

$$\forall \varepsilon > 0, U_X^\circ(\mathbf{x}, \varepsilon) \cap S \neq \emptyset.$$

Theorem 2.31. For a convergent sequence $\{\mathbf{x}_n : n \in \mathbb{N}, \forall i \neq j, \mathbf{x}_i \neq \mathbf{x}_j\} \subseteq X$, the point $x = \lim_{n \rightarrow \infty} \mathbf{x}_n$ is a cluster point of X .

Theorem 2.32. (Bolzano–Weierstrass Theorem) For a metric sapce X and a bounded infinite subset $S \subseteq X$, there exists at least one cluster point of X .

2.3 Normed Space

Definition 2.33. (Norm) For a linear space V over a field \mathbb{F} , the **norm** is a function $\|\cdot\| : V \rightarrow \mathbb{F}$ that satisfies

- (1) Positive definiteness: $\forall \mathbf{x} \in V, \|\mathbf{x}\| \geq 0, \|\mathbf{x}\| = 0 \Leftrightarrow \mathbf{x} = 0$,
- (2) Absolute homogeneity: $\forall \mathbf{x} \in V, k \in \mathbb{F}, \|k\mathbf{x}\| = |k| \|\mathbf{x}\|$,
- (3) Triangle inequality: $\forall \mathbf{x}, \mathbf{y} \in V, \|\mathbf{x}\| + \|\mathbf{y}\| \geq \|\mathbf{x} + \mathbf{y}\|$,

Definition 2.34. (Normed space) A **normed space** is a linear space V over the the field \mathbb{F} with a norm.

2.4 Inner Product Space

Definition 2.35. (Inner product) For a linear space V over a field \mathbb{F} , the **inner product** on V is a function $\langle \cdot, \cdot \rangle : V \times V \rightarrow \mathbb{F}$ that satisfies

- (1) Positive definiteness: $\forall \mathbf{x} \in V, \langle \mathbf{x}, \mathbf{x} \rangle \geq 0, \langle \mathbf{x}, \mathbf{x} \rangle = 0 \Leftrightarrow \mathbf{x} = 0$,
- (2) Conjugate symmetry: $\langle \mathbf{x}, \mathbf{y} \rangle = \overline{\langle \mathbf{y}, \mathbf{x} \rangle}$,
- (3) Linearity in the first argument: $\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in V, a, b \in \mathbb{F}, \langle a\mathbf{x} + b\mathbf{z}, \mathbf{y} \rangle = a\langle \mathbf{x}, \mathbf{y} \rangle + b\langle \mathbf{z}, \mathbf{y} \rangle$.

Definition 2.36. (Inner product space) An **inner product space** is a linear space V over the field \mathbb{F} with an inner product.

Theorem 2.37. Given a inner product space V and the norm defined as $\|\mathbf{x}\| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$ satisfies

$$\forall \mathbf{x}, \mathbf{y} \in V, \|\mathbf{x} + \mathbf{y}\|^2 + \|\mathbf{x} - \mathbf{y}\|^2 = 2 \|\mathbf{x}\|^2 + 2 \|\mathbf{y}\|^2.$$

2.4.1 Orthonormal system

Definition 2.38. A subset W of an inner product space V is called **orthonormal** if

$$\forall \mathbf{u}, \mathbf{v} \in S, \langle \mathbf{u}, \mathbf{v} \rangle = \begin{cases} 0, & u \neq v \\ 1, & u = v. \end{cases}$$

Definition 2.39. The **Gram-Schmidt process** takes in a finite or infinite independent list $(\mathbf{u}_1, \mathbf{u}_2, \dots)$ and output two other lists $(\mathbf{v}_1, \mathbf{v}_2, \dots)$ and $(\mathbf{u}_1^*, \mathbf{u}_2^*, \dots)$ by

$$\mathbf{v}_{n+1} = \mathbf{u}_{n+1} - \sum_{i=1}^n \langle \mathbf{u}_{n+1}, \mathbf{u}_i^* \rangle \mathbf{u}_i^*,$$

$$\mathbf{u}_{n+1}^* = \frac{\mathbf{v}_{n+1}}{\|\mathbf{v}_{n+1}\|},$$

with the recursion basis as $\mathbf{v}_1 = \mathbf{u}_1$.

Definition 2.40. Let $(\mathbf{u}_1^*, \mathbf{u}_2^*, \dots)$ be a finite or infinite orthonormal list. The **orthogonal expansion** or **Fourier expansion** for an arbitrary \mathbf{w} is the series

$$\sum_{i=1}^n \langle \mathbf{w}, \mathbf{u}_i^* \rangle \mathbf{u}_i^*,$$

where the constants $\langle \mathbf{w}, \mathbf{u}_i^* \rangle$ are known as the **Fourier coefficients** of \mathbf{w} and the term $\langle \mathbf{w}, \mathbf{u}_i^* \rangle \mathbf{u}_i^*$ is the **projection** of \mathbf{w} on \mathbf{u}_i^* .

Theorem 2.41. (Minimum properties of Fourier expansions) Let $\mathbf{u}_1^*, \mathbf{u}_2^*, \dots$ be an orthonormal system and let \mathbf{w} be arbitrary. Then

$$\forall a_1, \dots, a_n, \left\| \mathbf{w} - \sum_{i=1}^n \langle \mathbf{w}, \mathbf{u}_i^* \rangle \mathbf{u}_i^* \right\| \leq \left\| \mathbf{w} - \sum_{i=1}^n a_i \mathbf{u}_i^* \right\|,$$

where $\left\| \mathbf{w} - \sum_{i=1}^n a_i \mathbf{u}_i^* \right\|$ is minimized only when $a_i = \langle \mathbf{w}, \mathbf{u}_i^* \rangle$.

Theorem 2.42. (Bessel inequality) Let $\mathbf{u}_1^*, \mathbf{u}_2^*, \dots$ be an orthonormal system and let \mathbf{w} be arbitrary. Then

$$\sum_{i=1}^n |\langle \mathbf{w}, \mathbf{u}_i^* \rangle|^2 \leq \|\mathbf{w}\|^2.$$

2.5 Banach Space

Definition 2.43. (Banach space) A **Banach space** is a complete normed vector space.

2.6 Hilbert Space

Definition 2.44. (Hilbert space) A **Hilbert space** is a inner product space that is also complete with respect to the distance function induced by the inner product. a complete metric space.

2.7 Single Variable Polynomial

Definition 2.45. 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 2.46. 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 2.47. 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

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

Theorem 2.48. (Vieta's formulas) Given a polynomial $p \in \mathbb{P}_n$ with the coefficients being real or complex numbers, denoted by x_1, \dots, x_n the complex roots, then

$$\begin{cases} x_1 + \cdots + x_n = -c_{n-1}, \\ \sum_{i=1}^n \sum_{j=i+1}^n x_i x_j = c_{n-2}, \\ \quad \quad \quad \dots \\ \prod_{i=1}^n x_i = (-1)^n c_0, \end{cases}$$

where $c_n = 1$ WLOG.

2.8 Orthogonal Polynomial

Definition 2.49. 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 2.50. 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 ρ .

Theorem 2.51. The orthogonal polynomial $p_n(x)$ on $[a, b]$ with the weight function $\rho(x)$ has n roots on (a, b) .

2.8.1 Legendre polynomial

Definition 2.52. The **Legendre polynomial** is defined on $[-1, 1]$ with the weight function $\rho(x) = 1$.

Theorem 2.53. 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 2.54. The Legendre polynomial p_{n-1}, p_n, p_{n+1} satisfies

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

Example 2.55. The first three terms of Legendre polynomials is

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

2.8.2 Chebyshev polynomial of the first kind

Definition 2.56. 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 2.57. 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 2.58. 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 2.59. The first three terms of Chebyshev polynomials of the first kind is

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

2.8.3 Chebyshev polynomial of the second kind

Definition 2.60. The **Chebyshev polynomial of the second kind** is defined on $[-1, 1]$ with the weight function $\rho(x) = \sqrt{1-x^2}$.

Theorem 2.61. 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 2.62. 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 2.63. The first three terms of Chebyshev polynomials of the second kind is

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

2.8.4 Laguerre polynomial

Definition 2.64. The **Laguerre polynomial** is defined on $[0, +\infty)$ with the weight function $\rho(x) = x^\alpha e^{-x}$.

Theorem 2.65. 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 2.66. 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 2.67. For $\alpha = 0$, the first three terms of Laguerre polynomial is

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

2.8.5 Hermite polynomial (probability theory form)

Definition 2.68. 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 2.69. 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 2.70. 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 2.71. 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 3

Probability Theory

3.1 Discrete random variables

3.2 Continuous random variables

3.3 Characteristic functions

3.4 Probability limit theorems

Chapter 4

Stochastic Process

4.1 Poisson process

4.2 Markov chain

Chapter 5

Statistics

Chapter 6

Graph

6.1 Shortest Path

6.2 Matching

6.3 Network Flow

6.4 Tree

Chapter 7

Combinatorics

7.1 Generating function

7.2 Inclusion–exclusion principle

7.3 Special Numbers

7.3.1 Catalan number

7.3.2 Stirling number

Part 2

Scientific Computing

Chapter 8

Interpolation

8.1 Polynomial Interpolation

8.1.1 Lagrange formula

Definition 8.1. 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 $n = 0, l_0(x) = 1$.

8.1.2 Newton formula

Definition 8.2. The k th divided difference ($k \in \mathbb{N}^+$) on the **table of divided differences**

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

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 8.3. 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 8.4. 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 8.5. The **Newton formula** for interpolating the points $(x_0, f(x_0)), \dots, (x_n, f(x_n))$ is

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

8.1.3 Neville-Aitken algorithm

Definition 8.6. 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 .

8.1.4 Hermite interpolation

Definition 8.7. 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 8.8. (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 8.9. 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.

8.1.5 Approximation

Definition 8.10. 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 8.11. 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.

8.1.6 Error analysis

Theorem 8.12. 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 ξ depends on x, x_0, \dots, x_n and f .

Theorem 8.13. 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

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

8.2 Spline

Definition 8.14. 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.

8.2.1 Cubic spline

Definition 8.15. (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 8.16. 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 8.17. 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.

8.2.2 B-spline

Definition 8.18. 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 8.19. The $\{B_i^n(x)\}$ forms a basis of \mathbb{S}_n^{n-1} .

Definition 8.20. 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 8.21. (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 8.22. (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.

8.2.3 Error analysis

Theorem 8.23. 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 9

Integration

Definition 9.1. 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 9.2. 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 9.3. A weighted quadrature formula $I_n(f)$ satisfies $d_E \leq 2n - 1$.

Definition 9.4. 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 9.5. 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.

9.1 Newton-Cotes Formulas

Definition 9.6. A **Newton-Cotes formula** is a formula based on approximating $f(x)$ by interpolating it on uniformly spaced nodes $x_1, \dots, x_n \in [a, b]$.

9.1.1 Midpoint rule

Definition 9.7. 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 9.8. 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 9.9. The midpoint rule has $d_E = 1$.

9.1.2 Trapezoidal rule

Definition 9.10. 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 9.11. 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 9.12. The trapezoidal rule has $d_E = 1$.

9.1.3 Simpson's rule

Definition 9.13. 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 9.14. For $f \in C^4[a, b]$, with weight function $\rho \equiv 1$, the error (remainder) of Simpson's rule satisfies

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

Corollary 9.15. The Simpson's rule has $d_E = 3$.

9.2 Gauss Formulas

Theorem 9.16. 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 9.17. A Gauss formula $I_n(f)$ has $d_E = 2n - 1$.

Chapter 10

Optimization

10.1 One-dimensional Line Search

Definition 10.1. 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 10.2. (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 10.3. 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 α 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 10.4. 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 10.5. There is another **R-convergence** for judging a sequence which use another Q-convergence sequence as the boundary of $\{\|\mathbf{x}_k - \mathbf{x}^*\|\}$, but is not needed here.

Method 10.6. (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 10.7. The golden section method is a **linear convergent** method.

Method 10.8. (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 10.9. The Fibonacci method is a **linear convergent** method.

Method 10.10. (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 10.11. The bisection method is a **linear convergent** method.

Method 10.12. (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 10.13. The Newton's method is a **quadratic convergent** method.

10.2 Unconstrained Optimization

Definition 10.14. 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 α , 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 10.15. (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 α 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 10.16. The gradient descent method is a **linear convergent** method.

Method 10.17. (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 α_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 10.18. 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 10.19. The Quasi-Newton method is a **superlinear convergent** method.

Method 10.20. (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 α 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 10.21. The Newton's method is a **quadratic convergent** method.

Chapter 11

Initial Value Problem

Definition 11.1. 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 11.2. 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 $t_n = nk$.

11.1 Linear Multistep Method

Definition 11.3. 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 11.4. An LMM is **explicit** if $\beta_s = 0$, otherwise it is **implicit**.

11.2 Runge-Kutta Method

Definition 11.5. 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 11.6. 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 11.7. 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 11.8. 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.

11.3 Theoretical analysis

Definition 11.9. 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

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

11.3.1 Error analysis

Definition 11.10. The **local truncation error** τ is the error caused by replacing continuous derivatives with numerical formulas.

Definition 11.11. A numerical formulas is **consistent** if $\lim_{k \rightarrow 0} \tau = 0$.

11.3.2 Stability

Definition 11.12. 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 Ω that

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

Definition 11.13. 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 11.14. 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 11.15. A numerical method is **A(α)-stable** if the region of absolute stability Ω satisfies

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

Definition 11.16. A numerical method is **A-stable** if the region of absolute stability Ω satisfies

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

Definition 11.17. 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 11.18. An one-step method is **I-stable** iff its stability function satisfies

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

Definition 11.19. 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 11.20. 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 11.21. The order of accuracy of an implicit A-stable LMM satisfies $p \leq 2$. An explicit LMM cannot be A-stable.

Theorem 11.22. No ERK method is A-stable.

Theorem 11.23. 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 11.24. If an A-stable RK method with a nonsingular RK matrix A is stiffly accurate, then it is L-stable.

Theorem 11.25. 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 11.26. B-stable one-step methods are A-stable.

Theorem 11.27. An algebraically stable RK method is B-stable and A-stable.

11.3.3 Convergence

Definition 11.28. 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

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

Theorem 11.29. A numerical method is convergent iff it is consistent and stable.

11.4 Important Methods

11.4.1 Forward Euler's method

Definition 11.30. 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 11.31. The region of absolute stability for forward Euler's method is

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

11.4.2 Backward Euler's method

Definition 11.32. 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 11.33. The region of absolute stability for backward Euler's method is

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

11.4.3 Trapezoidal method

Definition 11.34. 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 11.35. The region of absolute stability for trapezoidal method is

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

11.4.4 Midpoint method (Leapfrog method)

Definition 11.36. 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 11.37. The region of absolute stability for midpoint method is

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

11.4.5 Heun's third-order RK method

Definition 11.38. The **Heun's third-order formula** is an ERK method of the form

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

11.4.6 Classical fourth-order RK method

Definition 11.39. The **classical fourth-order RK method** is an ERK method of the form

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

11.4.7 TR-BDF2 method

Definition 11.40. The **TR-BDF2 method** is an one-step method of the form

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

Chapter 12

Number Theory

12.1 Prime Number

Definition 12.1. A **prime number** (or a **prime**) is a natural number greater than 1 that is not a product of two smaller natural numbers.

Definition 12.2. A **composite number** (or a **composite**) is a natural number greater than 1 that is a product of two smaller natural numbers.

12.1.1 Primality testing

Theorem 12.3. For a integer $n \in \mathbb{N}$, if it is a product of two natural number a and b that $a \leq b$, then

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

Method 12.4. (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 12.5. (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 12.6. 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.

12.1.2 Sieves

Method 12.7. (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).

Part 3

Machine Learning

Chapter 13

Regression

13.1 Linear Regression

Definition 13.1. Given a data set $\{(\mathbf{x}_i, y_i), i \in \{1, \dots, m\}\}$ where $\mathbf{x}_i \in \mathbb{R}^n$, the linear regression seeks $\tilde{\mathbf{w}} \in \mathbb{R}^n$ and $\tilde{b} \in \mathbb{R}$ such that

$$f(\mathbf{x}_i) = \tilde{\mathbf{w}}^T \mathbf{x}_i + \tilde{b} \approx y_i.$$

In general, we choose mean square error to estimate the error between $f(\mathbf{x}_i)$ and y_i , which implies

$$(\tilde{\mathbf{w}}, \tilde{b}) = \arg \min_{\mathbf{w} \in \mathbb{R}^n, b \in \mathbb{R}} \sum_{i=1}^m (f(\mathbf{x}_i) - y_i)^2 = \arg \min_{\mathbf{w} \in \mathbb{R}^n, b \in \mathbb{R}} \sum_{i=1}^m (\mathbf{w}^T \mathbf{x}_i + b - y_i)^2.$$

Theorem 13.2. Given a data set $\{(\mathbf{x}_i, y_i), i \in \{1, \dots, m\}\}$ where $\mathbf{x}_i \in \mathbb{R}^n$, let

$$X = \begin{pmatrix} \mathbf{x}_1^T & 1 \\ \vdots & 1 \\ \mathbf{x}_m^T & 1 \end{pmatrix}, \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix},$$

if $X^T X$ is invertible, the solution of linear regression can be written as

$$\begin{pmatrix} \mathbf{w} \\ b \end{pmatrix} = (X^T X)^{-1} X^T \mathbf{y}.$$

Chapter 14

Decision Tree

Chapter 15

Support Vector Machine

Chapter 16

Cluster

Chapter 17

Neural Networks