Handbook of Applied Mathematics

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Part 1 Mathematical Foundation

Analysis

1.1 Calculus

1.1.1 Mean value theorem

Theorem 1.1. (Rolle's theorem) Given $n \ge 2$ and $f \in C^{n-1}([a,b])$ with $f^{(n)}(x)$ exists at each point of (a,b), suppose that $f(x_0) = \cdots f(x_n) = 0$ for $a \le x_0 < \cdots < x_n \le b$, then there is a point $\xi \in (a,b)$ such that $f^{(n)}(\xi) = 0$.

Theorem 1.2. (Lagrange's mean value theorem) Given $f \in C^1([a,b])$, then there exists $\xi \in (a,b)$ such that

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

Theorem 1.3. (Cauchy's mean value theorem) Given $f, g \in C^1([a, b])$, then there exists $\xi \in (a, b)$ such that

$$(f(b) - f(a))g'(\xi) = (g(b) - g(a))f'(\xi).$$

If $g(a) \neq g(b)$ and $g(\xi) \neq 0$, this is equivalent to

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

Theorem 1.4. (First mean value theorems for definite integrals) Given $f \in C([a,b])$ and g integrable and does not change sign on [a,b], then there exists ξ in (a,b) such that

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

Theorem 1.5. (Second mean value theorems for definite integrals) Given f a integrable function and g a positive monotonically decreasing function, then there exists ξ in (a,b) such that

$$\int_{a}^{b} f(x)g(x)dx = g(a) \int_{a}^{\xi} f(x)dx.$$

If g is a positive monotonically increasing function, then there exists ξ in (a,b) such that

$$\int_{a}^{b} f(x)g(x)dx = g(b) \int_{\varepsilon}^{b} f(x)dx.$$

If g is a monotonically function, then there exists ξ in (a,b) such that

$$\int_a^b f(x)g(x)dx = g(a)\int_a^{\xi} f(x)dx + g(b)\int_{\xi}^b f(x)dx.$$

1.1.2 Series

Definition 1.6. A series $\sum_{n=1}^{\infty} a_n$ is **absolute convergent** if the series of absolute values $\sum_{n=1}^{\infty} |a_n|$ converges.

Theorem 1.7. If a series is absolute convergent, then any reordering of it converges to the same limit.

Theorem 1.8. (n-th term test) If $\lim_{n\to\infty} a_n \neq 0$, then the series divergent.

Theorem 1.9. (Direct comparison test) If $\sum_{n=1}^{\infty} b_n$ is convergent and exists N>0, for all $n>N, \ 0\leq a_n\leq b_n$, then $\sum_{n=1}^{\infty} a_n$ is convergent; if $\sum_{n=1}^{\infty} b_n$ is divergent and exists N>0, for all $n>N, \ 0\leq b_n\leq a_n$, then $\sum_{n=1}^{\infty} a_n$ is divergent.

Theorem 1.10. (Limit comparison test) Given two series $\sum_{n=1}^{\infty} a_n$ and $\sum_{n=1}^{\infty} b_n$ with $a_n \ge 0$, $b_n > 0$. Then if $\lim_{n \to \infty} \frac{a_n}{b_n} = c \in (0, \infty)$, then either both series converge or both series diverge.

Theorem 1.11. (Ratio test) Given $\sum_{n=1}^{\infty} a_n$ and

$$R = \limsup_{n \to \infty} \left| \frac{a_{n+1}}{a_n} \right|, r = \liminf_{n \to \infty} \left| \frac{a_{n+1}}{a_n} \right|,$$

if R < 1, then the series converges absolutely; if r > 1, then the series diverges.

Theorem 1.12. (Root test) Given $\sum_{n=1}^{\infty} a_n$ and

$$R = \limsup_{n \to \infty} \left(|a_n| \right)^{\frac{1}{n}},$$

if R < 1, then the series converges absolutely; if R > 1, then the series diverges.

Theorem 1.13. (Integral test) Given $\sum_{n=1}^{\infty} f(n)$ where f is monotone decreasing, then the series converges iff the improper integral

$$\int_{1}^{\infty} f(x) \mathrm{d}x$$

is finite. In particular,

$$\int_{1}^{\infty} f(x) \mathrm{d}x \leq \sum_{n=1}^{\infty} f(n) \leq f(1) + \int_{1}^{\infty} f(x) \mathrm{d}x$$

Theorem 1.14. (Alternating series test) Given $\sum_{n=1}^{\infty} (-1)^n a_n$ where a_n are all positive or negative, then the series converges if $|a_n|$ decreases monotonically and $\lim_{n\to\infty} a_n = 0$.

1.1.3 Multivariable calculus

Theorem 1.15. (Green's theorem) Let Ω be the region in a plane with $\partial\Omega$ a positively oriented, piecewise smooth, simple closed curve. If P and Q are functions of (x,y) defined on an open region containing Ω and have continuous partial derivatives there, then

$$\oint_{\partial\Omega}(P\mathrm{d}x+Q\mathrm{d}y)=\iint_{\Omega}\bigg(\frac{\partial Q}{\partial x}-\frac{\partial P}{\partial y}\bigg)\mathrm{d}x\mathrm{d}y$$

where the path of integration along ${\cal C}$ is anticlockwise.

Theorem 1.16. (Stokes' theorem) Let Ω be a smooth oriented surface in \mathbb{R}^3 with $\partial\Omega$ a piecewise smooth, simple closed curve. If $\mathbf{F}(x,y,z) = \left(F_x(x,y,z), F_y(x,y,z), F_z(x,y,z)\right)$ is defined and has continuous first order partial derivatives in a region containing Ω , then

$$\iint_{\Omega} (\nabla \times \mathbf{F}) \cdot \mathrm{d}S(x) = \oint_{\partial \Omega} \mathbf{F} \cdot \mathrm{d}x$$

Theorem 1.17. (Gauss-Green theorem (Divergence theorem)) For a bounded open set $\Omega \in \mathbb{R}^n$ that $\partial \Omega \in C^1$ and a function $\mathbf{F}(\mathbf{x}) = (F_1(\mathbf{x}), ..., F_n(\mathbf{x})) : \overline{\Omega} \to \mathbb{R}^n$ 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 **n** is outward pointing unit normal vector at $\partial\Omega$.

Definition 1.18. An **implicit function** is a function of the form

$$F(x_1, ..., x_n) = 0,$$

where $x_1, ..., x_n$ are variables.

Theorem 1.19. Let $F(\mathbf{x}, \mathbf{y}) : \mathbb{R}^{n+m} \to \mathbb{R}^m$ be a differentiable function of two variables, and $(\mathbf{x}_0, \mathbf{y}_0)$ the point that $F(\mathbf{x}_0, \mathbf{y}_0) = \mathbf{0}$. If the Jacobian matrix

$$J_{F,\mathbf{y}}(\mathbf{x}_0,\mathbf{y}_0) = \left(\frac{\partial F_i}{\partial y_j}(\mathbf{x}_0,\mathbf{y}_0)\right)$$

is invertible, then there exists an open set $\Omega \subseteq \mathbb{R}^n$ containing \mathbf{x}_0 such that there exists a unique function $f: \Omega \to \mathbb{R}^m$ such that $f(\mathbf{x}_0) = \mathbf{y}_0$ and $F(\mathbf{x}, f(\mathbf{y})) = \mathbf{0}$ for all $\mathbf{x} \in \Omega$.

Moreover, f is continuously differentiable and, denoting the left-hand panel of the Jacobian matrix shown in the previous section as

$$J_{F,\mathbf{x}}(\mathbf{x}_0,\mathbf{y}_0) = \Bigg(\frac{\partial F_i}{\partial x_j}(\mathbf{x}_0,\mathbf{y}_0)\Bigg),$$

the Jacobian matrix of partial derivatives of f in Ω is given by

$$\left(\frac{\partial f_i}{\partial x_j}(\mathbf{x})\right)_{m \times n} = -\left(J_{F,\mathbf{y}}(\mathbf{x},f(\mathbf{x}))\right)_{m \times m}^{-1} \left(J_{F,\mathbf{x}}(\mathbf{x},f(\mathbf{x}))\right)_{m \times n}.$$

1.2 Important Inequalities

1.2.1 Fundamental inequality

Theorem 1.20. (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 1.21. (Triangle inequality)

$$a, b \in \mathbb{C}, \quad ||a| - |b|| \le |a \pm b| \le |a| + |b|,$$

 $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n, |\|\mathbf{a}\| - \|\mathbf{b}\|| \le \|\mathbf{a} \pm \mathbf{b}\| \le \|\mathbf{a}\| + \|\mathbf{b}\|.$

1.2.3 Bernoulli inequality

Theorem 1.22. (Bernoulli inequality)

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

1.2.4 Jensen's inequality

Theorem 1.23. (Jensen's inequality) For a real convex function $f(x):[a,b]\to\mathbb{R}$, numbers $x_1...,x_n\in[a,b]$ and weights $a_1,...,a_n$, the Jensen's inequality can be start as

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

And for concave function f,

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

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

1.2.5 Cauchy-Schwarz inequality

Theorem 1.24. (Cauchy-Schwarz inequality)

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

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

Equality holds iff $\frac{a_1}{b_1} = \cdots = \frac{a_n}{b_n}$ 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, $\forall \mathbf{a}, \mathbf{b} \in V \|\mathbf{a}\| \cdot \|\mathbf{b}\| \ge |\langle \mathbf{a}, \mathbf{b} \rangle|.$

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,

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

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

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

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

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 1.25. (Hölder's inequality)

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

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

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 $\frac{1}{p} + \frac{1}{q} = 1$,

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

1.2.7 Young's inequality

Theorem 1.26. (Young's inequality) For $p, q \in [1, +\infty)$ that $\frac{1}{p} + \frac{1}{q} = 1$,

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

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

1.2.8 Minkowski inequality

Theorem 1.27. (Minkowski inequality) For a metric space S,

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

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 1.28. 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 1.29. 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 1.30. A normal distribution or a Gaussian distribution is a continuous probability distribution of the form

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

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

1.3.2 Dirac delta function

Definition 1.31. The **Dirac delta function** centered at \overline{x} is

$$\delta(x-\overline{x}) = \lim_{\varepsilon \to 0} f_{\overline{x},\varepsilon}(x-\overline{x}),$$

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

Theorem 1.32. The Dirac delta function satisfies

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

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

Theorem 1.33. If $f: \mathbb{R} \to \mathbb{R}$ is continuous, then

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

1.3.3 Gamma function

Definition 1.34. The Gamma function defined on $\mathbb C$ is

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

where Re (z) > 0.

Theorem 1.35. The Gamma function satisfies

$$\forall x \in \mathbb{C}, \ \Gamma(x+1) = x\Gamma(x),$$

 $\forall n \in \mathbb{N}^*, \Gamma(n) = (n-1)!.$

Theorem 1.36. 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 1.37. 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 1.38. 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 1.39. The Beta function satisfies

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

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: $\forall \mathbf{x} \in V, \exists \mathbf{y} \in V, \text{ s.t. } \mathbf{x} + \mathbf{y} = 0,$
- (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: $\forall \mathbf{x}, \mathbf{y} \in V, a \in \mathbb{F}, a(\mathbf{x} + \mathbf{y}) = a\mathbf{x} + b\mathbf{y}$.

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

Definition 2.3. Denoted by $V_1, ..., V_n$ 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, ..., \mathbf{v}_n) : \mathbf{v}_1 \in V_1, ..., \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

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

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 $f:V\to W$ 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 $f \in \mathcal{L}(V, W)$, $f(\mathbf{0}) = f(0\mathbf{v}) = 0$.

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

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

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 $\operatorname{nullity}(f)$

Definition 2.12. For a linear map $f \in \mathcal{L}(V, W)$, the **image** of f is defined as $\operatorname{im}(f) = \{ \mathbf{w} \in W : \mathbf{w} = f(\mathbf{v}), \mathbf{v} \in V \},$

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

Theorem 2.13. (Rank-nullity theorem) For a linear map $f \in \mathcal{L}(V, W)$, $\dim(\ker(f)) + \dim(\inf(f)) = \dim(V)$.

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 $d: X \times X \to \mathbb{R}$ 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: $\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in V, d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z}) \ge d(\mathbf{x}, \mathbf{z}),$

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

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

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 $\{x_n\}$ 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

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

If it is decreased, then

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

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

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

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 $x = \lim_{n \to \infty} \mathbf{x}_n$ is a cluster point of X.

Theorem 2.32. (Bolzano-Weierstrass Theorem) For a metric sapce X and a bounded infinite subset $S \in X$, 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 $\|\cdot\|$: $V \to \mathbb{F}$ that satisfies

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

Definition 2.34. (Normed space) A normed space is a linear space V over 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 $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{F}$ 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 textsf{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 $(\mathbf{u}_1, \mathbf{u}_2, ...)$ and output two other lists $(\mathbf{v}_1, \mathbf{v}_2, ...)$ and $(\mathbf{u}_1^*, \mathbf{u}_2^*, ...)$ by

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

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

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

Definition 2.40. Let $(\mathbf{u}_1^*, \mathbf{u}_2^*, ...)$ 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

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

where $\|\mathbf{w} - \sum_{i=1}^{n} a_i \mathbf{u}_i^*\|$ 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

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

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 ce with respect to the distance function induced by the inner product 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 $c_0,...,c_n \in \mathbb{V}$ 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

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

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

$$\begin{cases} x_1 + \dots + x_n &= -c_{n-1}, \\ \sum\limits_{i=1}^n \sum\limits_{j=i+1}^n x_i x_j &= c_{n-2}, \\ & \dots \\ \prod\limits_{i=1}^n x_i &= (-1)^n c_0, \end{cases}$$

where $c_n = 1$ WLOG.

2.8 Orthogonal Polynomial

Definition 2.49. Given a weight function $\rho(x):[a,b]\to\mathbb{R}^+$, satisfies

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

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

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

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

$$\forall f,g \in L_{\rho}([a,b]), \langle f,g \rangle = \int_{a}^{b} \rho(x)f(x)g(x)\mathrm{d}x.$$

Theorem 2.50. Orthogonal polynomials $p_{n-1}(x), p_n(x), p_{n+1}(x)$ satisfies

$$p_{n+1}(x) = (a_n + b_n x) p_n(x) + c_n p_{n-1}(x). \label{eq:pn+1}$$

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

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

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

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

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

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

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

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

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

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

Theorem 2.66. For $\alpha=0$, the Laguerre polynomial p_{n-1},p_n,p_{n+1} satisfies $p_{n+1}(x)=(2n+1-x)p_n(x)-n^2p_{n-1}(x).$

Example 2.67. For $\alpha = 0$, the first three terms of Laguerre polynomial is $p_0(x) = 1$, $p_1(x) = -x + 1$, $p_2(x) = x^2 - 4x + 2$.

2.8.5 Hermite polynomial (probability theory form)

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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

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

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

Ordinary Differential Equation

Definition 3.1. Given a function F, an **explicit ordinary differential equation** of order n takes the form

$$\mathbf{F}(\mathbf{u}^{(n-1)},...,\mathbf{u}',\mathbf{u},t) = \mathbf{u}^{(n)},$$

an implicit ordinary differential equation of order n takes the form

$$\mathbf{F}\big(\mathbf{u}^{(n)},...,\mathbf{u}',\mathbf{u},t\big)=\mathbf{0},$$

Definition 3.2. An ODE is **autonomous** if it does not depend on the variable x.

Definition 3.3. A ODE is **linear** if can be written as

$$\sum_{i=0}^{n} A_i(t) \mathbf{u}^{(i)} + \mathbf{r}(t) = \mathbf{0},$$

where $A_i(t)$ and r(t) are continuous functions of t.

Definition 3.4. A linear ODE is **homogeneous** if $\mathbf{r}(t) = 0$, and there is always the trivial solution $\mathbf{u} \equiv \mathbf{0}$.

Definition 3.5. An ODE is **separable** if can be written as

$$P_1(x)Q_1(y) = P_2(x)Q_2(y)\frac{\mathrm{d}y}{\mathrm{d}x}.$$

Definition 3.6. For initial value $(\mathbf{u}_0, t_0) \in \mathbb{R}^n \times \mathbb{R}$, $T \geq t_0$ and $\mathbf{f} : \mathbb{R}^n \times [t_0, T] \to \mathbb{R}^n$, the **initial value problem** (IVP) is to find $u(t) \in C^1([t_0, T])$ satisfies

$$\mathbf{u}' = \mathbf{f}(\mathbf{u}, t), \quad \mathbf{u}(t_0) = \mathbf{u}_0.$$

Theorem 3.7. Given an IVP, denoted by $u_0 = u$, u_i , i = 1, ..., n the *i*th derivative of u, then the ODE

$$\mathbf{F}\big(\mathbf{u}^{(n-1)},...,\mathbf{u}',\mathbf{u},t\big) = \mathbf{u}^{(n)}$$

can be written as an IVP,

$$\begin{pmatrix} \mathbf{u}_0' \\ \vdots \\ \mathbf{u}_{n-2}' \\ \mathbf{u}_{n-1}' \end{pmatrix} = \begin{pmatrix} \mathbf{u}_1 \\ \vdots \\ \mathbf{u}_{n-1} \\ \mathbf{F}(\mathbf{u}_{n-1},...,\mathbf{u}_1,\mathbf{u}_0,t) \end{pmatrix}.$$

3.1 General Theory

Theorem 3.8. (Peano existence theorem) Given an IVP with an open set $\Omega \subseteq \mathbb{R}^n \times \mathbb{R}$, if $\mathbf{f}(\mathbf{u},t) \in C(\Omega)$ and $(\mathbf{u}_0,t_0) \in \Omega$, then there is a local solution $\tilde{\mathbf{u}}: U \to \mathbb{R}^n$ satisfies the IVP, where U is a neighbourhood of t_0 in \mathbb{R} .

Theorem 3.9. (Picard–Lindelöf theorem) Given an IVP with an open set $\Omega \subseteq \mathbb{R}^n \times \mathbb{R}$, if $\mathbf{f}(\mathbf{u},t): \Omega \to \mathbb{R}^n$ is continuous in t and Lipschitz continuous in \mathbf{u} and $(\mathbf{u}_0,t_0) \in \Omega$, then there is a unique local solution $\tilde{\mathbf{u}}: U \to \mathbb{R}^n$ satisfies the IVP, where U is a neighbourhood of t_0 in \mathbb{R} .

Theorem 3.10. (Comparison theorem) Given two IVPs

$$\mathbf{u}_1' = \mathbf{f}_1(\mathbf{u}_1, t), \quad \mathbf{u}_1(t_0) = \mathbf{u}_0,$$

$$\mathbf{u}_2' = \mathbf{f}_2(\mathbf{u}_2,t), \quad \mathbf{u}_2(t_0) = \mathbf{u}_0,$$

and a open set $\Omega \subseteq \mathbb{R}^n \times \mathbb{R}$, if for all $(\mathbf{u},t) \in \Omega$, $\mathbf{f}_1(\mathbf{u},t) < \mathbf{f}_2(\mathbf{u},t)$, then

$$\begin{cases} \mathbf{u}_1(t) > \mathbf{u}_2(t), & t > t_0, (\mathbf{u}_1(t), t), (\mathbf{u}_2(t), t) \in \Omega, \\ \mathbf{u}_1(t) < \mathbf{u}_2(t), & t < t_0, (\mathbf{u}_1(t), t), (\mathbf{u}_2(t), t) \in \Omega, \end{cases}$$

3.2 Exact solutions

Example 3.11. Given an initial point (y_0, x_0) , and a separable equation

$$P_1(x)Q_1(y) = P_2(x)Q_2(y)\frac{\mathrm{d}y}{\mathrm{d}x},$$

the solution of the equation is

$$\int_{x_0}^x \frac{P_1(t)}{P_2(t)}\mathrm{d}t = \int_{y_0}^y \frac{Q_2(t)}{Q_1(t)}\mathrm{d}t.$$

Example 3.12. Given an initial point (y_0, x_0) , and a first-order homogeneous equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} = F\left(\frac{y}{x}\right),$$

the solution of the equation is

$$\int_{x_0}^x \frac{1}{x} \mathrm{d}x = \int_{\frac{y_0}{x_0}}^{\frac{y}{x}} \frac{1}{F(t) - t} \mathrm{d}t.$$

Example 3.13. Given an initial point (y_0, x_0) , and a first-order separable equation

$$yM(xy) + xN(xy)\frac{\partial y}{\partial x} = 0,$$

the solution of the equation is

$$\int_{x_0}^{x} \frac{1}{x} \mathrm{d}x = \int_{y_0 x_0}^{yx} \frac{N(t)}{t(N(t) - M(t))} \mathrm{d}t,$$

where C is a constant.

Example 3.14. Given a nth-order, linear, inhomogeneous, constant coefficients equation

$$\sum_{i=0}^{n} a_i \frac{\partial^i y}{\partial x^i} = 0,$$

the solution of the equation is

$$\sum_{i=1}^k \left(\sum_{j=1}^{m_i} c_{ij} x^{j-1}\right) e^{\alpha_i x},$$

where $\left\{ c_{ij}\right\}$ are constants and α_{i} is the root of

$$\sum_{i=0}^{n} a_i x^i = 0$$

that repeated m_i times.

3.3 Important ODEs

3.3.1 Bernoulli differential equation

Definition 3.15. The Bernoulli differential equation takes the form

$$y' + P(x)y = Q(x)y^n,$$

where $n \neq 0, 1$.

Theorem 3.16. The solution of the Bernoulli differential equation is

$$y = (z(x))^{\frac{1}{1-n}},$$

where z(x) is the solution of

$$z' + (1-n)P(x)z + (1-n)Q(x) = 0.$$

3.3.2 Riccati equation

Definition 3.17. The Riccati equation takes the form

$$y' = q_0(x) + q_1(x)y + q_2(x)y^2,$$

where $q_0(x) \neq 0, q_2(x) \neq 0$.

Theorem 3.18. If u is one particular solution of the Riccati equation, the general solution is obtained as $y = u + \frac{1}{v}$, where v satisfies

$$v' + (q_1(x) + 2q_2(x)u)v + q_2(x).$$

Partial Differential Equation

Definition 4.1. A 2th order partial differential equation in \mathbb{R}^n takes the form

$$\sum_{i=0}^n \sum_{j=0}^n a_{ij}(\mathbf{x}) u_{x_i x_j} + \sum_{i=0}^n b_i(\mathbf{x}) u_{x_i} + c(\mathbf{x}) u(\mathbf{x}) = f(\mathbf{x}),$$

where $a_{ij}(\mathbf{x}) = a_{ji}(\mathbf{x})$.

Definition 4.2. Let $A(\mathbf{x}) = (a_{ij}(\mathbf{x}))_{n \times n}$ be a symmetric matrix, and $\lambda_1 \ge \cdots \ge \lambda_n$ the eigenvalues of A at \mathbf{x}_0 , then

- The equation is **elliptic** at \mathbf{x}_0 if for $i = 1, ..., n, \lambda_i < 0$
- The equation is **parabolic** at \mathbf{x}_0 if $\lambda_1 = 0$ and for $i = 2, ..., n, \lambda_i < 0$;
- The equation is **hyperbolic** at \mathbf{x}_0 if $\lambda_1 > 0$ and for $i = 2, ..., n, \lambda_i < 0$;

Definition 4.3. The boundary conditions for the unknown function y, constants c_0, c_1 specified by the boundary conditions, and known scalar functions g, h specified by the boundary conditions, where

- Dirichlet boundary condition: y = g;
- Neumann boundary condition: $\frac{\partial y}{\partial n} = g$; Robin boundary condition: $c_0 y + c_1 \frac{\partial y}{\partial n} = g$ where $c_0, c_1 \neq 0$;
- Mixed boundary condition: y = g and $c_0 y + c_1 \frac{\partial y}{\partial n} = h$ where $c_0, c_1 \neq 0$;
- Cauchy boundary condition: y = g and $\frac{\partial y}{\partial n} = h$.

Poisson's Equation 4.1

Definition 4.4. A **Poisson's equation** in \mathbb{R}^n takes the form

$$-\Delta u = f(\mathbf{x}),$$

where Δ is the Laplace operator, $u, f : \mathbb{R}^n \to \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^n$.

4.2Heat Equation

Definition 4.5. A Heat equation in $\mathbb{R}^n \times \mathbb{R}$ takes the form

$$\frac{\partial u}{\partial t} - a^2 \Delta u = f(\mathbf{x},t),$$

where Δ is the Laplace operator on \mathbb{R}^n , $u, f : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^n$.

Wave Equation

Definition 4.6. A Wave equation in $\mathbb{R}^n \times \mathbb{R}$ takes the form

$$\frac{\partial^2 u}{\partial t^2} - a^2 \Delta u = f(\mathbf{x}, t),$$

where Δ is the Laplace operator on \mathbb{R}^n , $u, f : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^n$.

Probability Theory

Definition 5.1. A probability space is a triple (Ω, \mathcal{F}, P) consisting of

- the sample space Ω : an arbitrary non-empty set;
- the σ -algebra $\mathcal{F} \subseteq 2^{\Omega}$: a set of subsets of Ω , called events, such that
 - \mathcal{F} contains the sample space: $\Omega \in \mathcal{F}$;
 - \mathcal{F} is closed under complements: if $A \in \mathcal{F}$, then also $(\Omega \setminus A) \in \mathcal{F}$;
 - \mathcal{F} is closed under countable unions: if $A_i \in \mathcal{F}, i=1,...$, then also $(\cup_{i=1}^{\infty} A_i) \in \mathcal{F}$;
- the probability measure $P:\mathcal{F}\to[0,1]$: a function such that
 - ▶ P is countably additive (also called σ-additive): if $\{A_i\}_{i=1}^{\infty} \subseteq \mathcal{F}$ is a countable collection of pairwise disjoint sets, then $P(\cup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} P(A_i)$;
 - the measure of the entire sample space is equal to one: $P(\hat{\Omega}) = 1$.

5.1 Characteristic functions

5.2 Probability limit theorems

Stochastic Process

- 6.1 Poisson process
- 6.2 Markov chain

Chapter 7
Statistics

Graph

- 8.1 Shortest Path
- 8.2 Matching
- 8.3 Network Flow
- **8.4** Tree

Combinatorics

- 9.1 Generating function
- 9.2 Inclusion-exclusion principle
- 9.3 Special Numbers
- 9.3.1 Catalan number
- 9.3.2 Stirling number

Part 2 Scientific Computing

Interpolation

10.1 Polynomial Interpolation

10.1.1 Lagrange formula

Definition 10.1. To interpolate given points $(x_0, f(x_0)), ..., (x_n, f(x_n))$, 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

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

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

10.1.2 Newton formula

Definition 10.2. The kth divided difference $(k \in \mathbb{N}^+)$ on the table of divided differences

where the divided differences satisfy

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

Corollary 10.3. Suppose $(i_0,...,i_k)$ is a permutation of (0,...,k). Then

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

Theorem 10.4. For distinct points $x_0, ..., x_n$ and x, we have

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

Definition 10.5. The **Newton formula** for interpolating the points $(x_0, f(x_0)), ..., (x_n, f(x_n))$ is

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

10.1.3 Neville-Aitken algorithm

Definition 10.6. Denote $p_0^{[i]}(x) = f(x_i)$ for i = 0, ..., n. For all k = 0, ..., n - 1 and i = 0, ..., n - k - 1, define

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

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

10.1.4 Hermite interpolation

Definition 10.7. Given distinct points $x_0, ..., x_k$ in [a, b], non-negative integers $m_0, ..., m_k$, and a function $f \in C^M[a, b]$ where $M = \max_{i=0,...,k} (m_i)$, the **Hermite interpolation problem** seeks a polynomial p(x) of the lowest degree satisfies

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

Definition 10.8. (Generalized divided difference) Let $x_0, ..., x_k$ 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 Nth divided difference associated with these points is the cofficient of x^N in the polynomial p that uniquely solves the Hermite interpolation problem.

Corollary 10.9. The nth divided difference at n+1 "confluent" (i.e. identical) points is

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

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

10.1.5 Approximation

Definition 10.10. Given condition functions $c_0, ..., c_k : \mathbb{P}_n \to \mathbb{R}^+$, the **Approximation problem** seeks a polynomial $p_n(x)$ of the given degree n satisfies a unconstrained optimization

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

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 10.11. For non-negative integers $m_0,...,m_k$ and condition functions $c_i(p_n) = \left(p_n^{(m_i)}(x)\right)^2$, denote by

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

the polynomial of the given degree n, then the mth 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.

10.1.6 Error analysis

Theorem 10.12. 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 $x_0, ..., x_n$. Define

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

as the Cauchy remainder of the polynomial interpolation.

If $a \le x_0 < \cdots < x_n \le b$, 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 $x, x_0, ..., x_n$ and f.

Theorem 10.13. 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

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

10.2 Spline

Definition 10.14. Given nonnegative integers n, k, and a strictly increasing sequence $a = x_1 < \cdots < x_N = b$, the set of **spline** functions of degree n and smoothness class k relative to the partition $\{x_i\}$ is

$$\mathbb{S}^k_n = \Big\{ s : s \in C^k[a,b]; \forall i \in \{1,...,N-1\}, s \mid_{[x_i,x_{i+1}]} \in \mathbb{P}_n \Big\},$$

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

10.2.1 Cubic spline

Definition 10.15. (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 10.16. Denote
$$m_i = s'(x_i), M_i = s''(x_i)$$
 for $s \in \mathbb{S}_3^2$, then $\forall i = 2, 3, ..., N-1, \quad \lambda_i m_{i-1} + 2m_i + \mu_i m_i + 1 = 3\mu_i f[x_i, x_{i+1}] + 3\lambda_i f[x_{i-1}, x_i],$ $\forall i = 2, 3, ..., N-1, \quad \mu_i M_{i-1} + 2M_i + \lambda_i m_{i+1} = 6f[x_{i-1}, x_i, x_{i+1}],$

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 10.17. 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.

10.2.2 B-spline

Definition 10.18. B-splines are defined recursively by

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

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

Definition 10.20. For $N \in \mathbb{N}^*$, the support of a $B_i^n(x)$ is

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

Theorem 10.21. (Integrals of B-splines) The average of a B-spline over its support only depends on its degree,

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

Theorem 10.22. (Derivatives of B-splines) For $n \geq 2$, we have

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

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.

10.2.3 Error analysis

Theorem 10.23. 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 $h = \max_{i=1,\dots,N-1} |x_{i+1} - x_i|$.

Integration

Definition 11.1. 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 $f \in C[a, b]$,

$$I(f) = \int_{a}^{b} \rho(x)f(x)\mathrm{d}x,$$

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 11.2. 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 11.3. A weighted quadrature formula $I_n(f)$ satisfies $d_E \leq 2n-1$.

Definition 11.4. 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

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

Theorem 11.5. Let $x_1,...,x_n$ be given as distinct nodes of $I_n(f)$. If $d_E \ge n-1$, then its weights can be deduced as

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

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

Newton-Cotes Formulas 11.1

Definition 11.6. A Newton-Cotes formula is a formula based on approximating f(x) by interpolating it on uniformly spaced nodes $x_1, ..., x_n \in [a, b]$.

11.1.1 Midpoint rule

Definition 11.7. 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

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

Theorem 11.8. For $f \in C^2[a, b]$, with weight functino $\rho \equiv 1$, the error (remainder) of midpoint rule satisfies

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

Corollary 11.9. The midpoint rule has $d_E = 1$.

11.1.2 Trapezoidal rule

Definition 11.10. 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 11.11. For $f \in C^2[a, b]$, with weight functino $\rho \equiv 1$, the error (remainder) of trapezoidal rule satisfies

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

Corollary 11.12. The trapezoidal rule has $d_E = 1$.

11.1.3 Simpson's rule

Definition 11.13. The **Simpson's rule** is a formula based on approximating f(x) by the quadratic polynomial that goes through the points $(a, f(a)), \left(\frac{a+b}{2}, f\left(\frac{a+b}{2}\right)\right)$ and (b, f(b)). For $\rho(x) \equiv 1$, it is simply

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

Theorem 11.14. For $f \in C^4[a, b]$, with weight functino $\rho \equiv 1$, 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 11.15. The Simpson's rule has $d_E = 3$.

11.2 Gauss Formulas

Theorem 11.16. For an interval [a, b] and a weight function $\rho : [a, b] \to \mathbb{R}$, 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 11.17. A Gauss formula $I_n(f)$ has $d_E = 2n - 1$.

Optimization

12.1 One-dimensional Line Search

Definition 12.1. Given a function $f : \mathbb{R}^n \to \mathbb{R}$, 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 12.2. (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 $a=\min\{\alpha,\alpha_k\}, \quad b=\max\{\alpha,\alpha_k\}.$

Definition 12.3. A general form of one-dimensional line search method is the following three steps:

- (1) **Initialization**: given initial point **x** and acceptable error $\varepsilon > 0$, $\delta > 0$;
- (2) **Iteration**: calculate the direction **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 $U_{\mathbb{R}^n}(x,\delta)$ 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 12.4. 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

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

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

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

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

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

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

Remark 12.5. 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 12.6. (Golden section method) Given the initial point 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 $b a \le \delta$;
- The solution is $\mathbf{x} + \frac{a+b}{2}\mathbf{d}$.

Theorem 12.7. The golden section method is a **linear convergent** method.

Method 12.8. (Fibonacci method) Given the initial point 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 $b a \le \delta$;
- The solution is $\mathbf{x} + \frac{a+b}{2}\mathbf{d}$.

Theorem 12.9. The Fibonacci method is a linear convergent method.

Method 12.10. (Bisection method) Given the initial point 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 $\nabla f(m) \cdot d < 0$, let a = m, otherwise let b = m.
- The stop condition is $b a \le \delta$;
- The solution is $\mathbf{x} + \frac{a+b}{2}\mathbf{d}$.

Theorem 12.11. The bisection method is a linear convergent method.

Method 12.12. (Newton's method) Given the initial point 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 12.13. The Newton's method is a quadratic convergent method.

12.2Unconstrained Optimization

Definition 12.14. Given a convex function $f: \mathbb{R}^n \to \mathbb{R}$, a unconstrained optimization method solves the problem

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

by

- (1) **Initialization**: given initial point **x** and acceptable error $\varepsilon > 0$, $\delta > 0$;
- (2) **Iteration**: calculate the direction **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 12.15. (Gradient descent method) Given the initial point 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 $\|\nabla f(\mathbf{x})\| \le \varepsilon$;
- The solution is \mathbf{x} .

Theorem 12.16. The gradient descent method is a linear convergent method.

Method 12.17. (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 12.18. 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

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

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 12.19. The Quasi-Newton method is a superlinear convergent method.

Method 12.20. (Newton's method) Given the initial point 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 $\|\nabla f(\mathbf{x})\| \le \varepsilon$;
- The solution is \mathbf{x} .

Theorem 12.21. The Newton's method is a quadratic convergent method.

Initial Value Problem

Notation 13.1. To numerically solve the IVP, we are given initial condition $\mathbf{u}_0 = \mathbf{u}(t_0)$, and want to compute approximations $\{\mathbf{u}_k, k = 1, 2, ...\}$ such that

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

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

13.1 Linear Multistep Method

Definition 13.2. For solving the IVP, an s-step **linear multistep method** (LMM) has the form

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

where $\alpha_s = 1$ is assumed WLOG.

Definition 13.3. An LMM is **explicit** if $\beta_s = 0$, otherwise it is **implicit**.

13.2 Runge-Kutta Method

Definition 13.4. An s-stage Runge-Kutta method (RK) is a one-step method of the form

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

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

Definition 13.5. The textsf{Butcher tableau} is one way to organize the coefficients of an RK method as follows

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

Definition 13.6. An s-stage **collocation method** is a numerical method for solving the IVP, where we

- (1) choose s distinct collocation parameters $c_1, ..., c_s$
- (2) seek s-degree polynomial p satisfying $\forall i = 1, 2, ..., s$, $\mathbf{p}(t_n) = \mathbf{u}_n$ and $\mathbf{p}'(t_n + c_i k) = \mathbf{f}(\mathbf{p}(t_n + c_i k), t_n + c_i k)$,
- (3) set $\mathbf{u}_{n+1} = \mathbf{p}(t_{n+1})$.

Theorem 13.7. The s-stage collocation method is an s-stage IRK method with

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

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

13.3 Theoretical analysis

Definition 13.8. A function $\mathbf{f}: \mathbb{R}^n \times [0, +\infty) \to \mathbb{R}^n$ is **Lipschitz continuous** in its first variable over some domain

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

iff

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

13.3.1 Error analysis

Definition 13.9. The local truncation error τ is the error caused by replacing continuous derivatives with numerical formulas.

Definition 13.10. A numerical formulas is **consistent** if $\lim_{k\to 0} \tau = 0$.

13.3.2 Stability

Definition 13.11. 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

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

Definition 13.12. The **stability function** of a one-step method is a function $R : \mathbb{C} \to \mathbb{C}$ that satisfies

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

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

Definition 13.13. 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

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

Definition 13.14. A numerical method is $\mathbf{A}(\alpha)$ -statble if the region of absolute stability Ω satisfies

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

Definition 13.15. A numerical method is **A-statble** if the region of absolute stability Ω satisfies

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

Definition 13.16. A one-step method is **L-stable** if it is A-stable, and its stability function satisfies

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

Definition 13.17. An one-step method is **I-stable** iff its stability function satisfies $\forall y \in \mathbb{R}, |R(y\mathbf{i})| \leq 1.$

Definition 13.18. 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

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

Definition 13.19. An RK method is **algebraically stable** iff the RK weights $b_1, ..., b_s$ 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 13.20. The order of accuracy of an implicit A-stable LMM satisfies $p \leq 2$. An explicit LMM cannot be A-stable.

Theorem 13.21. No ERK method is A-stable.

Theorem 13.22. 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 13.23. If an A-stable RK method with a nonsingular RK matrix A is stiffly accurate, then it is L-stable.

Theorem 13.24. If an A-stable RK method with a nonsingular RK matrix A satisfies

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

then it is L-stable.

Theorem 13.25. B-stable one-step methods are A-stable.

Theorem 13.26. An algebraically stable RK method is B-stable and A-stable.

13.3.3 Convergence

Definition 13.27. 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

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

Theorem 13.28. A numerical method is convergent iff it is consistent and stable.

13.4 Important Methods

13.4.1 Forward Euler's method

Definition 13.29. 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 13.30. The region of absolute stability for forward Euler's method is $\{z \in \mathbb{C} : |1+z| \le 1\}.$

13.4.2 Backward Euler's method

Definition 13.31. 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 13.32. The region of absolute stability for backward Euler's method is $\{z \in \mathbb{C} : |1-z| \geq 1\}.$

13.4.3 Trapezoidal method

Definition 13.33. 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 13.34. The region of absolute stability for trapezoidal method is

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

13.4.4 Midpoint method (Leapfrog method)

Definition 13.35. 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 13.36. The region of absolute stability for midpoint method is

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

13.4.5 Heun's third-order RK method

Definition 13.37. The **Heun's third-order formula** is an ERK method of the form

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

13.4.6 Classical fourth-order RK method

Definition 13.38. The classical fourth-order RK method is an ERK method of the form

$$\begin{cases} \mathbf{y}_{1} &= \mathbf{f}(\mathbf{u}_{n}, t_{n}), \\ \mathbf{y}_{2} &= \mathbf{f}\left(\mathbf{u}_{n} + \frac{k}{2}\mathbf{y}_{1}, t_{n} + \frac{k}{2}\right), \\ \mathbf{y}_{3} &= \mathbf{f}\left(\mathbf{u}_{n} + \frac{k}{2}\mathbf{y}_{2}, t_{n} + \frac{k}{2}\right), \\ \mathbf{y}_{4} &= \mathbf{f}(\mathbf{u}_{n} + k\mathbf{y}_{3}, t_{n} + k), \\ \mathbf{u}_{n+1} &= \mathbf{u}_{n} + \frac{k}{6}(\mathbf{y}_{1} + 2\mathbf{y}_{2} + 2\mathbf{y}_{3} + \mathbf{y}_{4}). \end{cases}$$

$$\begin{array}{c|cccc} \mathbf{0} & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \\ \end{array}$$

13.4.7 Third-order strong-stability preserving RK method

Definition 13.39. The third-order strong-stability preserving RK method is an ERK method of the form

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

which can also be written as

$$\begin{cases} \mathbf{y}_1 &= \mathbf{f}(\mathbf{u}_n, t_n), & 0 & 0 & 0 \\ \mathbf{y}_2 &= \mathbf{f}(\mathbf{u}_n + k\mathbf{y}_1, t_n + k), & 1 & 1 & 0 & 0 \\ \mathbf{y}_3 &= \mathbf{f}\left(\mathbf{u}_n + \frac{1}{4}k\mathbf{y}_1 + \frac{1}{4}k\mathbf{y}_2, t_n + \frac{1}{2}\right), & \frac{1}{2} & \frac{1}{4} & \frac{1}{4} & 0 \\ \mathbf{u}_{n+1} &= \mathbf{u}_n + \frac{k}{6}(\mathbf{y}_1 + \mathbf{y}_2 + 4\mathbf{y}_3). & \frac{1}{6} & \frac{1}{6} & \frac{2}{3} \end{cases}$$

13.4.8 TR-BDF2 method

Definition 13.40. The TR-BDF2 method is an one-step method of the form

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

Number Theory

14.1 Prime Number

Definition 14.1. A **prime number** (or a **prime**) is a natural number greater than 1 that is not a product of two smaller natural numbers.

Definition 14.2. A **composite number** (or a **composite**) is a natural number greater than 1 that is a product of two smaller natural numbers.

14.1.1 Primality testing

Theorem 14.3. For a integer $n \in \mathbb{N}$, if it is a product of two natural number a and b than $a \leq b$, then

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

Method 14.4. (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 14.5. (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 14.6. 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 $a^u, a^{u \times 2}, a^{u \times 2^2}, ..., a^{u \times 2^{t-1}}$;
- (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.

14.1.2 Sieves

Method 14.7. (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: $\{2, 3, 4, ..., n\}$;
- (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

Regression

15.1 Linear Regression

Definition 15.1. Given a data set $\{(\mathbf{x}_i, y_i), i \in \{1, ..., m\}\}$ 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

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

Theorem 15.2. Given a data set $\{(\mathbf{x}_i, y_i), i \in \{1, ..., m\}\}$ 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^TX is invertible, the solution of linear regression can be written as

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

Chapter 16
Decision Tree

Chapter 17 Support Vector Machine

Cluster

18.1 K-means

Definition 18.1. Given points $\mathbf{x}_1,...,\mathbf{x}_m \in \mathbb{R}^n$, **k-means clustering** aims to partition the points into $k \leq n$ sets $S = \{S_1,...,S_k\}$ satisfies

$$S = \operatorname*{arg\,min}_{S} \bigg\{ \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} \lVert \mathbf{x} - \mathbf{\mu}_i \rVert^2 \bigg\},$$

where μ_i is the mean (centroid) of points in S_i , i.e. denoted by $|S_i|$ the size of S_i ,

$$\mu_i = \frac{1}{|S_i|} \sum_{\mathbf{x} \in S_i} \mathbf{x}.$$

Theorem 18.2. Denoted by $\mathbf{x}_1,...,\mathbf{x}_m \in \mathbb{R}^n$ the points and $S = \{S_1,...,S_k\}$ sets given by K-means,

$$S = \mathop{\arg\min}_{S} \Biggl\{ \sum_{i=1}^{k} \frac{1}{|S_i|} \sum_{\mathbf{x}, \mathbf{y} \in S_i} \lVert \mathbf{x} - \mathbf{y} \rVert^2 \Biggr\}.$$

Method 18.3. (K-means clustering) Denoted by $S^{(t)} = \left\{S_1^{(t)}, ..., S_k^{(t)}\right\}$ the sets given by k-means at t-th step and $\mu_i^{(t)}$ the mean of $S_i^{(t)}$, the algorithm proceeds by

(1) Assignment: Assign each point to the cluster with the nearest mean,

$$S_i^{(t)} = \left\{\mathbf{x}_p : \forall j \in \{1,...,k\}, \|\mathbf{x}_p - \mathbf{\mu}_i^{(t)}\|^2 \leq \|\mathbf{x}_p - \mathbf{\mu}_j^{(t)}\|^2\right\};$$

(2) Update: Recalculate means (centroids) of each cluster,

$$\mu_i^{(t)} = \frac{1}{|S_i^{(t)}|} \sum_{\mathbf{x} \in S_i^{(t)}} \mathbf{x}.$$

Chapter 19 Neural Networks