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Part 1 Mathematical Foundation

Chapter 1

Analysis

1.1 Calculus

Definition 1.1. A number x is a **lower bound** of a nonempty set S if $\forall s \in S, x \leq s$.

Definition 1.2. A number x is a **upper bound** of a nonempty set S if $\forall s \in S, x \geq s$.

Definition 1.3. Let S be a nonempty set, denoted by $\inf S$ the **infimum** of S where

- (1) $\forall s \in S, s \ge \inf S$;
- (2) $\forall y > \inf S, \exists s \in S \text{ s.t. } s < y.$

Definition 1.4. Let S be a nonempty set, denoted by $\inf S$ the supremum of S where

- (1) $\forall s \in S, s \leq \sup S$;
- (2) $\forall y < \sup S, \exists s \in S \text{ s.t. } s > y.$

Theorem 1.5. Let $S_1 \subseteq S_2$, then $\inf S_1 \ge \inf S_2$, $\sup S_1 \le \sup S_2$.

Corollary 1.6. $\inf \emptyset = +\infty, \sup \emptyset = -\infty.$

Theorem 1.7. A set Ω is **closed** if it contains all the limits of convergent sequences of points in Ω .

Definition 1.8. A set Ω is bounded if there exists $R \in \mathbb{R}^+$ such that $\Omega \subseteq \{\mathbf{x} \in \mathbb{R}^n : ||\mathbf{x}|| \le R\}$.

Theorem 1.9. (Bolzano-Weierstrass) Let $\Omega \subset \mathbb{R}^n$ a bounded closed set. If $\left\{\mathbf{x}^{[k]}\right\}_{k=1}^{\infty} \subseteq \Omega$, then there exists $\mathbf{x}^* \in \Omega$ and a subsequence $\left\{\mathbf{x}^{[k_i]}\right\}_{i=1}^{\infty}$ such that

$$\lim_{i \to \infty} \mathbf{x}^{[k_i]} = \mathbf{x}^*.$$

Definition 1.10. A bounded closed set in \mathbb{R}^n is called a **compact set**.

Theorem 1.11. Let Ω be a nonempty set and $f \in C(\Omega)$, then f achieves its infimum and supremum over Ω , i.e.

$$\exists x,y \in \Omega, f(x) = \inf_{\Omega} f, f(y) = \sup_{\Omega} f.$$

Theorem 1.12. (Rolle's theorem) Let $f \in C([a,b]) \cap C^1((a,b))$, if f(a) = f(b), then there exists a point $\xi \in (a,b)$ such that $f'(\xi) = 0$.

Theorem 1.13. (Generalized 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), if $f(x_0) = \cdots f(x_n) = 0$ for $a \le x_0 < \cdots < x_n \le b$, then there exists a point $\xi \in (a,b)$ such that $f^{(n)}(\xi) = 0$.

Theorem 1.14. (Taylor's theorem with remainder term) Let f be n+1 times differentiable on an open interval containing [a, b], then there exists $\xi \in (a, b)$,

$$f(b) = \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!} (b-a)^k + \frac{f^{(n+1)}(\xi)}{(n+1)!} (b-a)^{n+1}$$

Theorem 1.15. (High-dimensional Taylor's theorem with remainder term) Let $f \in C^1(\mathbb{R}^n)$, $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, then there exists $\xi \in (0,1)$ such that

$$f(\mathbf{y}) = f(\mathbf{x}) + (\nabla f((1-\xi)\mathbf{x} + \xi\mathbf{y}))^T(\mathbf{y} - \mathbf{x}).$$

Let $f \in C^2(\mathbb{R}^n)$, $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, then there exists $\xi \in (0,1)$ such that

$$f(\mathbf{y}) = f(\mathbf{x}) + (\nabla f(\mathbf{x}))^T (\mathbf{y} - \mathbf{x}) + (\mathbf{y} - \mathbf{x})^T \nabla^2 f((1 - \xi)\mathbf{x} + \xi \mathbf{y})(\mathbf{y} - \mathbf{x}).$$

Theorem 1.16. Let $f \in C^2(\mathbb{R}^n)$ and there exists L such that $L \ge \|\nabla^2 f(\mathbf{x})\|_2$ for all $x \in \mathbb{R}^n$, then

$$\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n, \|\nabla f(u) - \nabla f(v)\|_2 \leq L \|\mathbf{u} - \mathbf{v}\|_2.$$

Theorem 1.17. Let $h \in C^2(\mathbb{R}^m)$ and let $A \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^m$. Define f(x) = h(Ax - b) then $f \in C^2(\mathbb{R}^n)$ and $\nabla f(x) = A^T \nabla h(Ax - b)$, $\nabla^2 f(x) = A^T \nabla^2 h(Ax - b)A$.

Theorem 1.18. (Subdifferential inequality) Let h be convex C^1 , then

$$\forall x,y \in \mathbb{R}^n, h(y) - h(x) \ge (\nabla h(x))^T (y - x).$$

1.1.1 Generalized derivative

Definition 1.19. (Generalized derivative) For $f(x) \in L^1_{loc}(\Omega)$, then $g(x) \in L^1_{loc}(\Omega)$ is called the $|\alpha|$ -th order generalized derivative of f(x) if

$$\forall \varphi(x) \in C^{\alpha}(\Omega), \int_{\Omega} g(x)\varphi(x)\mathrm{d}x = (-1)^{|\alpha|} \int_{\Omega} f(x)\partial^{\alpha}\varphi(x)\mathrm{d}x,$$

with the notation

$$D^{\alpha} f(x) = q(x).$$

Theorem 1.20. If $f(x) \in C^{\alpha}(\Omega)$, then $D^{\alpha}f(x) = f^{\alpha}(x)$.

Theorem 1.21. Given $\Omega = \Omega_1 \cup \Omega_1$, $m(\Omega_1 \cap \Omega_1) = 0$, and $f \in C(\overline{\Omega}) \cap C^1(\Omega_1) \cap C^1(\Omega_2)$, then $D^{\alpha}f(x)$ exists for $|\alpha| = 1$, and for all $x \in \text{int } \Omega_1 \cup \text{int } \Omega_2$, $D^{\alpha}f(x) = f^{\alpha}(x)$.

1.1.2 Convex sets and functions

Definition 1.22. A set $\Omega \subseteq \mathbb{R}^n$ is said to be **convex** if for any $\mathbf{x}, \mathbf{y} \in \Omega$, and $\lambda \in (0, 1)$, it holds that $\lambda \mathbf{x} + (1 - \lambda)\mathbf{y} \in \Omega$.

Theorem 1.23. Let $\Omega \subseteq \mathbb{R}^n$ be a nonempty closed convex set and $\mathbf{y} \in \mathbb{R}^n$, then there exists a unique solution to the following optimization problem:

$$\min_{\mathbf{x} \in \mathbb{R}^n} \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|_2 \quad \text{s.t.} \quad \mathbf{x} \in \Omega.$$

The unique solution is called the projection of \mathbf{y} onto Ω , denoted by $P_{\Omega}(y)$.

Theorem 1.24. Let $\Omega \subset \mathbb{R}^n$ be a nonempty closed convex set, $\mathbf{y} \in \mathbb{R}^n$ and $\mathbf{u} \in \Omega$, then

$$(\mathbf{y} - P_{\Omega}(\mathbf{y}))^{T} (\mathbf{u} - P_{\Omega}(\mathbf{y})) \le 0.$$

Theorem 1.25. (Separation) Let $\Omega \subseteq \mathbb{R}^n$ be a nonempty closed convex set and $\mathbf{y} \in \mathbb{R}^n \setminus \Omega$, then there exists $\mathbf{v} \in \mathbb{R}^n \setminus \{0\}$ and $\alpha \in \mathbb{R}$ so that

$$\mathbf{v}^T \mathbf{y} > \alpha > \mathbf{v}^T \mathbf{u}$$

for all $\mathbf{u} \in \Omega$.

Theorem 1.26. Let $A \in \mathbb{R}^{m \times n}$, then the set $S = \{A\mathbf{y} : \forall i = 1, ..., n, \mathbf{y}_i \geq 0\}$ is closed and convex.

Definition 1.27. A function $f: \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ is called

- Proper if $dom(f) = {\mathbf{x} : f(x) < \infty} \neq \emptyset$;
- Convex if $\operatorname{epi}(f) = \{(\mathbf{x}, r) : r \ge f(\mathbf{x})\}\$ is convex;
- Closed if is lower semicontinuous $\underline{\lim}_{\mathbf{x}\to\mathbf{x}_0} f(\mathbf{x}) \geq f(\mathbf{x}_0)$ (same as $\mathrm{epi}(f)$ is closed).

Theorem 1.28. Let $f: \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$, it is convex iff for any $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$ and $\lambda \in (0,1)$, it holds that

$$f(\lambda \mathbf{u} + (1 - \lambda)\mathbf{v}) \le \lambda f(\mathbf{u}) + (1 - \lambda)f(\mathbf{v}).$$

Theorem 1.29. (First-order condition under convexity) Let $f \in C^1(\mathbb{R}^n)$, if f is convex and $\nabla f(\mathbf{x}) = 0$, then \mathbf{x} is a global minimizer of f.

Theorem 1.30. Let $f \in C^2(\mathbb{R}^n)$, then f is convex iff $\nabla^2 f(\mathbf{x}) \succeq 0$ for all $\mathbf{x} \in \mathbb{R}^n$.

Proposition 1.31. Let $f: \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$, $g: \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ both be convex, $A \in \mathbb{R}^{n \times p}$, $b \in \mathbb{R}^n$, $H(\mathbf{x}) = A\mathbf{x} - b$ and $\alpha > 0$, then the following functions are convex:

$$f + g$$
, αf , $f \circ H = f(A\mathbf{x} - \mathbf{b})$, $\max\{f, g\}$, $\|\cdot\|$.

Proposition 1.32. Let $f: \mathbb{R}^n \to [0, +\infty)$ and $g: [0, +\infty) \to \mathbb{R}$ both be convex and non-decreasing, then $g \circ f = g(f(\mathbf{x}))$ is convex.

1.1.3 Mean value theorem

Theorem 1.33. (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 1.34. (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 1.35. (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 1.36. (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

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

Theorem 1.37. (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

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

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

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

1.1.4 Series

Definition 1.38. 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 1.39. If a series is absolute convergent, then any reordering of it converges to the same limit.

Theorem 1.40. (n-th term test) If $\lim_{n\to\infty} a_n \neq 0$, then the series divergent.

Theorem 1.41. (Direct comparison test) If $\sum_{n=1}^{\infty} b_n$ is convergent and exists N > 0, for all n > N, $0 \le a_n \le b_n$, 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, $0 \le b_n \le a_n$, then $\sum_{n=1}^{\infty} a_n$ is divergent.

Theorem 1.42. (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 1.43. (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 1.44. (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 1.45. (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,

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

Theorem 1.46. (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 $\lim_{n\to\infty} a_n = 0$.

1.1.5 Multivariable calculus

Theorem 1.47. (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 C is anticlockwise.

Theorem 1.48. (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 1.49. (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 1.50. An **implicit function** is a function of the form

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

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

Theorem 1.51. 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 Real Analysis

1.2.1 Lebesgue Measure

Definition 1.52. Given an bounded interval $I \in \mathbb{R}$, denoted by $\mathcal{E}(I)$ the **length** of the interval defined as the distance of its endpoints,

$$\mathscr{E}([a,b]) = \mathscr{E}((a,b)) = b - a.$$

Definition 1.53. For any subset $E \subset \mathbb{R}$, the **Lebesgue outer measure** $m^*(E)$ is defined as

$$m^*(E) = \inf \Biggl\{ \sum_{i=1}^n \mathscr{C}(I_i) : \left\{ I_i \right\}_{i=1}^n \ \text{ is a sequence of open intervals that } \ E \subset \bigcup_{i=1}^n I_i \Biggr\}.$$

Theorem 1.54. If $E_1 \subset E_2 \subset \mathbb{R}$, then $m^*(E_1) \leq m^*(E_2)$.

Theorem 1.55. Given an interval $I \subset \mathbb{R}$, $m^*(I) = \ell(I)$.

Theorem 1.56. Given $\{E_i \subset \mathbb{R}\}_{i=1}^n$, $m^*\left(\bigcup_{i=1}^n E_i\right) \leq \sum_{i=1}^n m^*(E_i)$.

Definition 1.57. The sets E are said to be **Lebesgue-measurable** if

$$\forall A \subset \mathbb{R}, m^*(A) = m^*(A \cap X) + m^*(A \cap (\mathbb{R} \setminus A))$$

and its Lebesgue measure is defined as its Lebesgue outer measure: $m(E) = m^*(E)$.

Theorem 1.58. The set of all measurable sets $E \subset \mathbb{R}$ forms a σ -algebra \mathcal{F} where

- \mathcal{F} contains the sample space: $\mathbb{R} \in \mathcal{F}$;
- \mathcal{F} is closed under complements: if $A \in \mathcal{F}$, then also $(\mathbb{R} \setminus A) \in \mathcal{F}$;
- \mathcal{F} is closed under countable unions: if $A_i \in \mathcal{F}, i=1,...$, then also $(\bigcup_{i=1}^{\infty} A_i) \in \mathcal{F}$.

Definition 1.59. A measurable space is a tuple (X, \mathcal{F}) consisting of an arbitrary non-empty set X and a σ -algebra $\mathcal{F} \subseteq 2^X$.

1.3 Complex Analysis

Definition 1.60. Given an open set Ω and a function $f(z):\Omega\to\mathbb{C}$, the **derivative** of f(z) at a point $z_0\in\Omega$ is defined as the limits

$$f'(z) = \lim_{z \to z_0} \frac{f(z) - f(z_0)}{z - z_0},$$

and the function is said to be **complex differentiable** at z_0 .

Definition 1.61. A function f(z) is holomorphic on an open set Ω if it is complex differentiable at every point of Ω .

Theorem 1.62. If a complex function $f(x + \mathbf{i}y) = u(x, y) + \mathbf{i}v(x, y)$ is holomorphic, then u and v have first partial derivatives, and satisfy the Cauchy–Riemann equations,

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}$$
 and $\frac{\partial u}{\partial y} = \frac{\partial v}{\partial x}$,

or equivalently,

$$\frac{\partial f}{\partial \overline{z}} = 0.$$

Theorem 1.63. (Cauchy's integral theorem) Given a simply connected domain Ω and a holomorphic function f(z) on it, for any simply closed contour C in Ω ,

$$\int_C f(z) \mathrm{d}x = 0.$$

Theorem 1.64. (Residue formula) Suppose that f is holomorphic in an open set containing a toy contour γ and its interior, except for some points $z_1, ..., z_n$ inside γ , then

$$\int_{\gamma} f(z) dz = 2\pi \mathbf{i} \sum_{k=1}^{n} \operatorname{res}_{z_{k}} f,$$

where for a pole z_0 of order n,

$$\operatorname{res}_{z_0} f = \lim_{z \to z_0} \frac{1}{(n-1)!} \bigg(\frac{\mathrm{d}}{\mathrm{d}z}\bigg)^{n-1} (z-z_0)^n f(z).$$

1.4 Important Inequalities

1.4.1 Fundamental inequality

Theorem 1.65. (Fundamental inequality)

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

1.4.2 Triangle inequality

Theorem 1.66. (Triangle inequality)

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

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

1.4.3 Bernoulli inequality

Theorem 1.67. (Bernoulli inequality)

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

1.4.4 Jensen's inequality

Theorem 1.68. (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

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

And for concave function f,

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

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

1.4.5 Cauchy-Schwarz inequality

Theorem 1.69. (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 $\frac{a_1}{b_1} = \dots = \frac{a_n}{b_n}$ 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,

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

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).

1.4.6 Hölder's inequality

Theorem 1.70. (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 $\frac{1}{p} + \frac{1}{q} = 1$,

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

1.4.7 Young's inequality

Theorem 1.71. (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 $a^p = b^q$.

1.4.8 Minkowski inequality

Theorem 1.72. (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.

1.4.9 Friedriches inequality

Theorem 1.73. (Friedriches inequality) Given a bounded simply connected region $\Omega \subset \mathbb{R}^n$, with the diameter d, then for $u \in H_0^1(\Omega)$,

$$||u||_{L^2(\Omega)} \le d||\nabla u||_{L^2(\Omega)}.$$

1.5 Special Functions

1.5.1 Gaussian function

Definition 1.74. 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 1.75. 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 1.76. A **normal distribution** or a **Gaussian distribution** is a continuous probability distribution of the form

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

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

1.5.2 Dirac delta function

Definition 1.77. 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 1.78. 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 1.79. If $f: \mathbb{R} \to \mathbb{R}$ is continuous, then

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

1.5.3 Gamma function

Definition 1.80. 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 1.81. 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 1.82. The Gamma function satisfies

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

which implies

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

1.5.4 Beta Function

Definition 1.83. For $p, q \in \mathbb{R}^+$, the **Beta function** is defined as

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

Theorem 1.84. 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 1.85. The Beta function satisfies

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

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

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

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

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 $f \in \mathcal{L}(V, W)$,

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

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

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 $\{x_n\}$ 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. (Equivalent norms) Two norms $p(\cdot), q(\cdot)$ on \mathbb{R}^n are called equivalent if

$$\exists C_1, C_2 \in \mathbb{R}^+ \quad \text{s.t.} \quad \forall \mathbf{x} \in V, C_1 q(\mathbf{x}) \leq p(\mathbf{x}) \leq C_2 q(\mathbf{x}).$$

Definition 2.35. (Normed space) A normed space is a linear space V over the field \mathbb{F} with a norm.

2.3.1 Vector norm and matrix norm

Example 2.36. The followings are some commonly used vector norms:

- (1) l_1 norm: $\|\mathbf{x}\|_1 = \sum_{i=1}^n |\mathbf{x}_i|;$
- (2) $l_2 \text{ norm: } \|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^n |\mathbf{x_i}|^2};$
- (3) l_{∞} norm: $\|\mathbf{x}\|_{\infty} = \max_{1 \leq i \leq n} |\mathbf{x}_i|$.

Theorem 2.37. Any two l_p norms $\|\cdot\|_p$, $\|\cdot\|_q$ on \mathbb{R}^n are equivalent.

Example 2.38. For l_p norms on \mathbb{R}^n ,

$$\|\mathbf{x}\|_{2} \leq \|\mathbf{x}\|_{1} \leq \sqrt{n} \|\mathbf{x}\|_{2}, \ \|\mathbf{x}\|_{\infty} \leq \|\mathbf{x}\|_{2} \leq \sqrt{n} \|\mathbf{x}\|_{\infty}, \ \|\mathbf{x}\|_{\infty} \leq \|\mathbf{x}\|_{1} \leq n \|\mathbf{x}\|_{\infty}.$$

Definition 2.39. Let $\left\{\mathbf{x}^{[k]} \in \mathbb{R}^n\right\}_{i=1}^{\infty}$ be a sequences and $\mathbf{x}^* \in \mathbb{R}^n$, then

$$\lim_{i \to \infty} \mathbf{x}^{[i]} = \mathbf{x}^* \Leftrightarrow \forall 1 \le k \le n, \lim_{i \to \infty} \mathbf{x}_k^{[i]} = \mathbf{x}_k^*.$$

Corollary 2.40. Let $\|\cdot\|$ be a norm on \mathbb{R}^n , $\left\{\mathbf{x}^{[i]}\right\}_{i=1}^{\infty} \subset \mathbb{R}^n$ be a sequences and $x^* \in \mathbb{R}^n$, then

$$\lim_{i \to \infty} \mathbf{x}^{[k]} = \mathbf{x}^* \Leftrightarrow \lim_{i \to \infty} \left\| \mathbf{x}^{[k]} - \mathbf{x}^* \right\| = 0.$$

Definition 2.41. A function $\|\cdot\|: \mathbb{R}^{n \times n} \to \mathbb{R}$ is called a **matrix norm** if

- (1) Positive definiteness: $\forall A \in \mathbb{R}^{n \times n}, ||A|| \ge 0, ||A|| = 0$ iff A = 0;
- (2) Absolute homogeneity: $\forall A \in \mathbb{R}^{n \times n}, k \in \mathbb{R}, ||kA|| = |k|||A||$;
- (3) Triangle inequality: $\forall A, B \in \mathbb{R}^{n \times n}, ||A|| + ||B|| \ge ||A + B||;$
- (4) Sub-multiplicative: $\forall A, B \in \mathbb{R}^{n \times n}, ||A|| ||B|| \ge ||AB||$.

Theorem 2.42. Let $\|\cdot\|$ be a vector norm, then the matrix norm induced by the vector norm can be written as

$$\|A\| = \max_{\mathbf{x} \in \mathbb{R}^n} \frac{\|A\mathbf{x}\|}{\|\mathbf{x}\|} = \max_{\|\mathbf{x}\|=1} \|A\mathbf{x}\|.$$

Example 2.43. The followings are some commonly used matrix norms:

- (1) $\|A\|_1 = \max_j \sum_{i=1}^n |a_{ij}|$ (maximum of the l_1 norms of columns);
- (2) $||A||_2 = \sqrt{\lambda_{\max}(A^T A)};$
- (3) $\|A\|_{\infty} = \max_{i} \sum_{j=1}^{n} |a_{ij}|$ (maximum of the l_1 norms of rows);
- (4) $||A||_F = \sqrt{\sum_{i=1}^n \sum_{j=1}^n a_{ij}^2}$ (Frobenius norm).

Definition 2.44. Let $A \in \mathbb{R}^{n \times n}$ be symmetric, then A is **positive semidefinite** if $\mathbf{x}^T A \mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$, A is **positive definite** if $\mathbf{x}^T A \mathbf{x} > 0$ for all $\mathbf{x} \in \mathbb{R}^n$.

Notation 2.45. We write $A \succeq 0$ if A is positive semidefinite, $A \succ 0$ if A is positive definite. The set of $n \times n$ positive semidefinite matrices is denoted by S^n_+ .

Theorem 2.46. Let $A \in \mathbb{R}^{n \times n}$ be symmetric, then the following statements are equivalent

- (1) All eigenvalues of A are nonnegative;
- (2) There exists $M \in \mathbb{R}^{n \times n}$ such that $A = M^T M$;
- (3) A is positive semidefinite.

Theorem 2.47. Let $A \in \mathbb{R}^{n \times n}$ be symmetric, then the following statements are equivalent

- (1) All eigenvalues of A are positive;
- (2) There exists an invertible matrix $M \in \mathbb{R}^{n \times n}$ such that $A = M^T M$;

(3) A is positive definite.

Remark 2.48. Let $A \succ 0$, then

- (1) $A^{-1} \succ 0$ and $\lambda_{\min}(A) = \inf\{\mathbf{x}^T A \mathbf{x} : \|\mathbf{x}\|_2 = 1\};$
- (2) $||A||_2 = \lambda_{\max}(A) = (\lambda_{\min}(A^{-1}))^{-1}$.

2.4 Inner Product Space

Definition 2.49. (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 2.50. (Inner product space) An inner product space is a linear space V over the field \mathbb{F} with an inner product.

Theorem 2.51. 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 2.52. 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 2.53. 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

$$\begin{split} \mathbf{v}_{n+1} &= \mathbf{u}_{n+1} - \sum_{i=1}^n \langle \mathbf{u}_{n+1}, \mathbf{u}_k^* \rangle \mathbf{u}_k^*, \\ \mathbf{u}_{n+1}^* &= \frac{\mathbf{v}_{n+1}}{\|\mathbf{v}_{n+1}\|}, \end{split}$$

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

Definition 2.54. 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 2.55. (Minimum properties of Fourier expansions) Let $\mathbf{u}_1^*, \mathbf{u}_2^*, ...$ 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 2.56. (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 2.57. (Banach space) A Banach space is a complete normed vector space.

2.6 Hilbert Space

Definition 2.58. (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 2.59. 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 2.60. 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 2.61. 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 2.62. (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 2.63. Given a weight function $\rho(x):[a,b]\to\mathbb{R}^+$, 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

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

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

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

Theorem 2.64. 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 2.65. 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 2.66. The **Legendre polynomial** is defined on [-1,1] with the weight function $\rho(x) = 1$.

Theorem 2.67. 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 2.68. 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 2.69. 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 2.70. 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 2.71. 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 2.72. 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 2.73. 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 2.74. The Chebyshev polynomial of the second kind is defined on [-1,1] with the weight function $\rho(x) = \sqrt{1-x^2}$.

Theorem 2.75. 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 2.76. 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 2.77. 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 2.78. The **Laguerre polynomial** is defined on $[0, +\infty)$ with the weight function $\rho(x) = x^{\alpha}e^{-x}$.

Theorem 2.79. 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 2.80. 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 2.81. 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)

Definition 2.82. 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 2.83. 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 2.84. 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 2.85. For $\alpha = 0$, the first three terms of Hermite polynomial is

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

Chapter 3

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

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

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 *n*th-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

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

Chapter 4

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 $\lambda_1 \geq \cdots \geq \lambda_n$ 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 $\frac{\partial y}{\partial n} = h$.

4.1 Poisson's Equation

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 $\mathbf{x} \in \mathbb{R}^n$.

4.2 Heat 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 $\mathbf{x} \in \mathbb{R}^n$.

4.3 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 $\mathbf{x} \in \mathbb{R}^n$.

Chapter 5

Probability Theory

Probability 5.1

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 $(\bigcup_{i=1}^{\infty} A_i) \in \mathcal{F}$;
- 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 $P(\bigcup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} P(A_i)$;
 - the measure of the entire sample space is equal to one: $P(\Omega) = 1$.

Definition 5.2. Given a probability space (Ω, \mathcal{F}, P) , a random variable is a measurable function $X: \Omega \to \mathbb{R}$ that for all $t \in \mathbb{R}$,

$$\{\omega \in \Omega : X(\omega) \le t\} \in \mathcal{F}.$$

Definition 5.3. The cumulative distribution function (cdf) of a random variable X on probability space (Ω, \mathcal{F}, P) is

$$F_X(x) = P(X \le x).$$

Continuous random variables

Definition 5.4. A continuous random variables is a random variables with the range of X is uncountable.

Definition 5.5. The probability density function (pdf) of a continuous random variables is

$$f(x) = \frac{\mathrm{d}F(x)}{\mathrm{d}x}.$$

Theorem 5.6. Let X be a discrete random variables, its probability mass function satisfies

- (1) $f(x) \ge 0$;
- (2) $\int_{-\infty}^{+\infty} f(x) dx = 1;$ (3) $F(x) = \int_{-\infty}^{x} f(t) dt.$

Theorem 5.7. Let X be a continuous random variables and Y = g(X) is a differentiable bijection, denoted by $f_X(x), f_Y(y)$ the pdf's of X and Y, then

$$f_Y(y) = f_X(g^{-1}(y)) \left| \frac{\mathrm{d}x}{\mathrm{d}y} \right|.$$

5.1.2 Discrete random variables

Definition 5.8. A discrete random variables is a random variables with the range of X is countable.

Definition 5.9. The **probability mass function (pmf)** of a discrete random variables is

$$p_{X(x)} = P(X = x).$$

Theorem 5.10. Let X be a discrete random variables, its probability mass function satisfies

$$0 \leq p_X(x) \leq 1 \text{ and } \sum_{x \in \text{Range}(X)} p_X(x) = 1.$$

Theorem 5.11. Let X be a discrete random variables and Y = g(X), denoted by $p_X(x), p_Y(y)$ the pmf's of X and Y, then

$$p_Y(y) = \sum_{x; q(x) = y} p_X(x).$$

In particular, if g is a bijection, then

$$p_Y(y) = p_X(g^{-1}(y)).$$

Remark 5.12. The discrete random variable X can be written in continuous form via Dirac delta function, i.e.

$$f_X(x) = \sum_{\overline{x} \in \, \operatorname{Range}(X)} p_X(x) \delta(x - \overline{x}).$$

5.1.3 Multivariate distributions

Definition 5.13. A random vector is a vector $(X_1, ..., X_n)$ where all X_k are random variables.

Definition 5.14. The **joint cdf** of a random vector $(X_1,...,X_n)$ is defined as

$$F_{X_1,...,X_n}(x_1,...,x_n) = P(X_1 \leq x_1,...,X_n \leq x_n).$$

Definition 5.15. The **joint pmf** of a random vector $(X_1,...,X_n)$ is defined as

$$p_{X_1,...,X_n}(x_1,...,x_n) = P(X_1 = x_1,...,X_n = x_n).$$

Definition 5.16. The **joint pdf** of a random vector $(X_1,...,X_n)$ is defined as

$$f_{X_1,\dots,X_n}(x_1,\dots,x_n) = \frac{\partial F_{X_1,\dots,X_n}(x_1,\dots,x_n)}{\partial x_1 \cdots \partial x_n}.$$

Theorem 5.17. A random vector $(X_1, ..., X_n)$ satisfies

$$(1)\ \ F_{X_1,...,X_{n-1}}(x_1,...,x_{n-1})=F_{X_1,...,X_n}(x_1,...,x_{n-1},+\infty);$$

(2)
$$p_{X_1,\dots,X_{n-1}}(x_1,\dots,x_{n-1}) = \sum_{x \in \, \mathrm{Range}(X_n)} p_{X_1,\dots,X_n}(x_1,\dots,x_{n-1},x)$$
 (discrete case);

- $(3) \ \ f_{X_1,\dots,X_{n-1}}(x_1,\dots,x_{n-1}) = \int_{-\infty}^{+\infty} f_{X_1,\dots,X_n}(x_1,\dots,x_{n-1},x) \mathrm{d}x \quad \text{(continuous case)};$
- $(4) \ \ p_{X_1,\dots,X_n \ | \ X_1}(x_1,\dots,x_n \ | \ x_1) = \frac{p_{X_1,\dots,X_n}(x_1,\dots,x_n)}{p_{X_1}(x_1)} \quad \text{(discrete case)};$ $(5) \ \ f_{X_1,\dots,X_n \ | \ X_1}(x_1,\dots,x_n \ | \ x_1) = \frac{f_{X_1,\dots,X_n}(x_1,\dots,x_n)}{f_{X_1}(x_1)} \quad \text{(continuous case)}.$

Theorem 5.18. Given two random vectors $X=(X_1,...,X_n)$ and $Y=(Y_1,...,Y_n)$ and a series of bijection $\{g_i\}$ that $X_i = g_{i(Y_i)}$, then

$$f_{Y_1,\dots,Y_n}(y_1,\dots,y_n) = f_{X_1,\dots,X_n}(g_1(y_1,\dots,y_n),\dots,g_n(y_1,\dots,y_n)) \left| \frac{\partial (x_1,\dots,x_n)}{\partial (y_1,\dots,y_n)} \right|.$$

Theorem 5.19. Two random vectors $X = (X_1, ..., X_n)$ and $Y = (Y_1, ..., Y_n)$ are mutually independent iff

$$\begin{cases} p_{X_1,X_2}(x_1,x_2) = p_{X_1}(x_1)p_{X_2}(x_2), & \text{(discrete case)}, \\ f_{X_1,X_2}(x_1,x_2) = f_{X_1}(x_1)f_{X_2}(x_2), & \text{(continuous case)}. \end{cases}$$

Distributional quantities 5.1.4

Definition 5.20. Given a random variable X, the **expectation** of X is

$$E(X) = \sum_{x \in \, \mathrm{Range}(X)} x p(x), \quad \mathrm{if} \, \sum_{x \in \, \mathrm{Range}(X)} |x| p(x) < \infty \qquad \, (\mathrm{discrete \,\, case})$$

$$E(X) = \int_{-\infty}^{+\infty} x f(x) dx, \quad \text{if } \int_{-\infty}^{+\infty} |x| f(x) dx < \infty \quad \text{(continuous case)}.$$

Definition 5.21. Given a random variable X, the k-th moment of X is $E(X^k)$, and the kth central moment is $E((X - E(X))^k)$.

Example 5.22. The variance of random variable X is the **2-nd central moment** of X,

$$\sigma^2=\operatorname{Var}(X)=E\big((X-E(X))^2\big)=E\big(X^2\big)-E(X)^2.$$

Definition 5.23. Given a random variable X, if $E(e^{tX})$ exists for $t \in \mathbb{R}$, then the moment generating function (mgf) of X is

$$M_X(t) = E(e^{tX}) = \sum_{k=0}^{\infty} \frac{t^k E\big(X^k\big)}{k!}.$$

Theorem 5.24. The moment generating function (mgf) of random variables X and Y satisfies

- (1) For all $k \in \mathbb{N}^*$, $M^{(k)}(0) = E(X^k)$;
- (2) If X and Y are independent, then $M_{X+Y}(t) = M_X(t)M_Y(t)$.

Characteristic functions

Probability limit theorems 5.3

Common distributions

5.4.1 Common discrete distributions

Definition 5.25. (Bernoulli distribution) If X is a random variable with Bernoulli $(p), p \in (0,1)$, then:

$$P(X = 1) = p, P(X = 0) = 1 - p.$$

Theorem 5.26. For Bernoulli(p), the expectation is $\mu = p$, the variance is $\sigma^2 = p(1-p)$, the moment generating function is $M(t) = (1-p) + pe^t$.

Definition 5.27. (Binomial distribution) If X is a random variable with Binomial $(n, p), p \in (0, 1), n \in \mathbb{N}^*$, then:

$$P(X = x) = C_n^x p^x (1-p)^{n-x}, x = 0, 1, ..., n.$$

Theorem 5.28. For Binomial(n, p), the expectation is $\mu = np$, the variance is $\sigma^2 = np(1-p)$, the moment generating function is $M(t) = ((1-p) + pe^t)^n$.

Definition 5.29. (Geometric distribution) If X is a random variable with Geometric $(p), p \in (0,1)$, then:

$$P(X = x) = p(1 - p)^x, x \in \mathbb{N}.$$

Theorem 5.30. For Geometric(p), the expectation is $\mu = \frac{p}{1-p}$, the variance is $\sigma^2 = \frac{1-p}{p^2}$, the moment generating function is $M(t) = p(1-(1-p)e^t)^{-1}$.

Definition 5.31. (Hypergeometric distribution) If X is a random variable with Hypergeometric (N, D, n), $n = 1, 2, ..., \min(N, D)$, then:

$$P(X = x) = \frac{C_{N-D}^{n-x}C_D^x}{C_N^n}, x = 0, 1, ..., n.$$

Theorem 5.32. For Hypergeometric (N, D, n), the expectation is $\mu = \frac{nD}{N}$, the variance is $\sigma^2 = \frac{nD(N-D)(N-n)}{N^2(N-1)}$.

Definition 5.33. (Negative binomial distribution) If X is a random variable with $NB(r, p), r \in \mathbb{N}^*, p \in (0, 1)$, then:

$$P(X = x) = C_{x+r-1}^{r-1} p^r (1-p)^x, x \in \mathbb{N}.$$

Theorem 5.34. For NB(p), the expectation is $\mu = \frac{rp}{1-p}$, the variance is $\sigma^2 = \frac{r(1-p)}{p^2}$, the moment generating function is $M(t) = p^r (1 - (1-p)e^t)^{-r}$.

Definition 5.35. (Poisson distribution) If X is a random variable with Poisson(λ), $\lambda > 0$, then:

$$P(X = x) = e^{-\lambda} \frac{\lambda^x}{x!}, x \in \mathbb{N}.$$

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Theorem 5.36. For Poisson(p), the expectation is $\mu = \lambda$, the variance is $\sigma^2 = \lambda$, the moment generating function is $M(t) = \exp(\lambda(e^t - 1))$.

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

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

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

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

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

$$\begin{split} &\forall i=2,3,...,N-1, \quad \lambda_i m_{i-1} + 2m_i + \mu_i m_i + 1 = 3\mu_i f\big[x_i,x_{i+1}\big] + 3\lambda_i f\big[x_{i-1},x_i\big], \\ &\forall i=2,3,...,N-1, \quad \mu_i M_{i-1} + 2M_i + \lambda_i m_{i+1} = 6f\big[x_{i-1},x_i,x_{i+1}\big], \end{split}$$

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

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

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 $h = \max_{i=1,\dots,N-1} \lvert x_{i+1} - x_i \rvert.$

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

$$\begin{aligned} &\forall f \in \mathbb{P}_{d_E}, \quad E_n(f) = 0, \\ &\exists g \in \mathbb{P}_{d_E+1}, \text{ s.t. } E_n(g) \neq 0 \end{aligned}$$

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.

11.1 Newton-Cotes Formulas

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

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

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

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

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

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 $(a, f(a)), (\frac{a+b}{2}, f(\frac{a+b}{2}))$ and (b, f(b)).

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

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

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

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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 nth 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 Optimality Conditions

Definition 12.1. Let $f : \mathbb{R}^n \to \mathbb{R}$, \mathbf{x}^* is a global minimizer of f if $\forall \mathbf{x} \in \mathbb{R}^n$, $f(\mathbf{x}) \geq f(\mathbf{x}^*)$. Let $f : \mathbb{R}^n \to \mathbb{R}$, \mathbf{x}^* is a local minimizer of f if $\exists \delta > 0$, $\forall \mathbf{x} \in U(\mathbf{x}, \delta)$, $f(\mathbf{x}) \geq f(\mathbf{x}^*)$.

Theorem 12.2. (1st-order necessary conditions) Let $f \in C^1(\mathbb{R}^n)$ and \mathbf{x}^* be a local minimizer of f, then $\nabla f(\mathbf{x}^*) = 0$.

Definition 12.3. Let $f \in C^1(\mathbb{R}^n)$ then \mathbf{x}^* is called a stationary point of f if $\nabla f(\mathbf{x}^*) = 0$.

Theorem 12.4. (2nd-order necessary conditions) Let $f \in C^2(\mathbb{R}^n)$.

- If \mathbf{x}^* is a local minimizer of f, then $\nabla^2 f(\mathbf{x}^*) \succeq 0$;
- If \mathbf{x}^* is a stationary point of f and $\nabla^2 f(\mathbf{x}^*) \succ 0$, then \mathbf{x}^* is a local minimizer.

Definition 12.5. Let $f \in C^1(\mathbb{R}^n)$ and $\mathbf{x} \in \mathbb{R}^n$. A $\mathbf{d} \in \mathbb{R}^n$ is called a **descent direction** at x if $(\nabla f(\mathbf{x}))^T \mathbf{d} < 0$.

Specifically, $-\nabla f(x)$ is called the **steepest descent direction**.

Remark 12.6. Let $D \in \mathbb{R}^{n \times n}$ and $D \succ 0$, then $d = -D\nabla f(x)$ is a descent direction.

12.1.1 KKT Conditions

Definition 12.7. We say that x^* is a local minimizer of

$$\begin{split} \min_{x \in \mathbb{R}^n} f(x) \\ \text{s.t.} \quad h_j(x) = 0, j = 1, ..., p, \\ g_i(x) \leq 0, i = 1, ..., m. \end{split}$$

if x^* is feasible and exists $\varepsilon > 0$ such that $f(x) \ge f(x^*)$ whenever x is feasible and $\|x - x^*\|_2 \le \varepsilon$.

Theorem 12.8. (Karush-Kuhn-Tucker conditions for the LP, KKT condition) Consider the linear program

$$\min_{x \in \mathbb{R}^n} c^T x$$
 s.t. $Bx = d$,
$$Ax \le b$$
.

where $c \in \mathbb{R}^n$, $B \in \mathbb{R}^{p \times n}$ and $A \in \mathbb{R}^{q \times n}$. Then $x^* \in \mathbb{R}^n$ is an optimal solution iff there exists $\lambda^* \in \mathbb{R}^q$ and $\mu^* \in \mathbb{R}^p$ such that the following conditions holds:

- (Primal feasibility) $Bx^* = d$ and $Ax \leq b$;
- (Dual feasibility) $B^T \mu^* + A^T \lambda^* + c = 0$ and $\lambda^* \ge 0$;

• (Complementary slackness) $\lambda^{*^T}(Ax^* - b) = 0$.

Theorem 12.9. (Mangasarian-Fromovitz constraint qualification) Consider the feasible set of

$$\begin{aligned} & \min_{x \in \mathbb{R}^n} f(x) \\ & \text{s.t.} & h_j(x) = 0, j = 1, ..., p, \\ & q_i(x) < 0, i = 1, ..., m. \end{aligned}$$

and let x^* be feasible. We say that the Mangasarian-Fromovitz constraint qualification (MFCQ) holds at x^* if the following conditions holds:

• If $\sum_{j\in J} \mu_j \nabla h_j(x^*) + \sum_{i\in I(x^*)} \lambda_i \nabla g_i(x^*) = 0$ and $\forall i\in I(x^*), \lambda_i \geq 0$ then $\lambda_i = 0$ for all $i\in I(x^*)$ and $\mu_j = 0$ for all $j\in J$.

Theorem 12.10. (KKT conditions for NLP) Consider

$$\begin{aligned} & \min_{x \in \mathbb{R}^n} f(x) \\ & \text{s.t.} & h_j(x) = 0, j = 1, ..., p, \\ & g_i(x) \leq 0, i = 1, ..., m. \end{aligned}$$

and let x^* be a local minimizer. Suppose that MFCQ holds at x^* . Then there exists $\lambda^* \in \mathbb{R}^m$ and $\mu^* \in \mathbb{R}^p$ such that

•
$$\nabla f(x^*) + \sum_{j \in J} \mu_j^* \nabla h_j(x^*) + \sum_{i \in I(x^*)} \lambda_i^* \nabla g_i(x^*) = 0$$
 and $\forall i \in I, \lambda_i^* \geq 0, \lambda_i^* g_i(x^*) = 0$.

Definition 12.11. Consider

$$\begin{aligned} & \min_{x \in \mathbb{R}^n} f(x) \\ & \text{s.t.} & h_j(x) = 0, j = 1, ..., p, \\ & g_i(x) \leq 0, i = 1, ..., m. \end{aligned}$$

An \overline{x} is called a stationary point if it is feasible and there exist $\overline{\lambda} \in \mathbb{R}^m$ and $\overline{\mu} \in \mathbb{R}^p$ such that

•
$$\nabla f(\overline{x}) + \sum_{j \in J} \overline{\mu_j} \nabla h_j(\overline{x}) + \sum_{i \in I(\overline{x})} \overline{\lambda_i} \nabla g_i(\overline{x}) = 0$$
 and $\forall i \in I, \overline{\lambda_i} \geq 0, \overline{\lambda_i} g_i(\overline{x}) = 0$.

Theorem 12.12. (MFCQ from Slater) Consider the set defined by

$$S = \{x \in \mathbb{R}^n : \forall i \in I, g_i(x) \le 0\},\$$

where g_i are convex C^1 . Suppose that there exist \overline{x} satisfying

$$\forall i \in I, g_i(\overline{x}) < 0.$$

Then MFCQ holds at every point in S.

Theorem 12.13. (MFCQ from generalized Slater) Consider the set defined by

$$S = \{ x \in \mathbb{R}^n : \forall i \in I, g_i(x) \le 0, Ax = b \},$$

where g_i are convex C^1 and $A \in \mathbb{R}^{p \times n}$. Suppose that there exist \overline{x} satisfying

$$\forall i \in I, g_i(\overline{x}) < 0, A\overline{x} = b,$$

and A has full row rank. Then MFCQ holds at every point in S.

Theorem 12.14. (Sufficiency under convexity) Consider

$$\begin{aligned} & \min_{x \in \mathbb{R}^n} \quad f(x) \\ & \text{s.t.} \quad Ax = b, \\ & g_i(x) \leq 0, i \in I, \end{aligned}$$
 where f and g_i are convex $C^1, A \in \mathbb{R}^{p \times n}$.

Suppose that there exist $x^* \in \mathbb{R}^n$, $\lambda^* \in \mathbb{R}^m$ and $\mu^* \in \mathbb{R}^p$ such that

- $\forall i \in I, g_i(x^*) \leq 0, Ax^* = b;$
- $$\begin{split} \bullet \quad & \nabla f(x^*) + \sum_{i \in I} \lambda_i^* \nabla g_i(x^*) + A^T \mu^* = 0; \\ \bullet \quad & \forall i \in I, \lambda_i^* \geq 0, \lambda_i^* g_i(x^*) = 0. \end{split}$$

Then x^* is a global minimizer.

One-dimensional Line Search 12.2

Inexact line search 12.2.1

Definition 12.15. (Armijo rule) Let $\sigma \in (0,1)$, $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{d} \in \mathbb{R}^n$. Find $\alpha > 0$ such that

$$f(\mathbf{x} + \alpha \mathbf{d}) \le f(\mathbf{x}) + \alpha \sigma (\nabla f(\mathbf{x}))^T \mathbf{d}.$$

Theorem 12.16. Let $f \in C^1(\mathbb{R}^n)$, $\mathbf{x} \in \mathbb{R}^n$, $\sigma \in (0,1)$ and $\mathbf{d} \in \mathbb{R}^n$ be a descent direction at \mathbf{x} . Then there exists $\alpha_1 > 0$ such that for all $\alpha \in [0, \alpha_1]$,

$$f(\mathbf{x} + \alpha \mathbf{d}) \le f(\mathbf{x}) + \alpha \sigma (\nabla f(\mathbf{x}))^T \mathbf{d}.$$

Method 12.17. (Armijo line search by backtracking) Fix $\sigma \in (0,1)$ and $\beta \in (0,1)$. Given $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{d} \in \mathbb{R}^n$ and $\overline{\alpha} > 0$. Find the smallest nonnegative integer j such that

$$f(\mathbf{x} + \overline{\alpha}\beta^j \mathbf{d}) \le f(\mathbf{x}) + \overline{\alpha}\beta^j \sigma(\nabla f(\mathbf{x}))^T \mathbf{d},$$

then the stepsize generated is $\overline{\alpha}\beta^{j}$.

Theorem 12.18. (Convergence under Armijo rule) Let $f \in C^1(\mathbb{R}^n)$ with $\inf f > -\infty$. Let $\{\overline{\alpha}^{[k]}\}\subset \mathbb{R}$ satisfies $0<\inf_k\alpha^{[k]}\leq \sup_k\alpha^{[k]}<\infty$, and fix $\sigma\in(0,1)$ and $\beta\in(0,1)$. Suppose $\{\mathbf{x}^{[k]}\}$ is generated as $\mathbf{x}^{[k+1]} = \mathbf{x}^{[k]} + \alpha^{[k]}\mathbf{d}^{[k]}$, where

- $\mathbf{d}^{[k]} = -D^{[k]}\nabla f(\mathbf{x}^{[k]})$, where $\{D^{[k]}\}$ is a bounded sequence of positive definite matrices with $D^{[k]} - \delta I \succ 0$ for some δ :
- $\alpha^{[k]}$ is generated via the Armijo line search by backtracking.

Then any accumulation point of $\{x^{[k]}\}$ is a stationary point of f.

Definition 12.19. (Wolfe's condition) Let $0 < c_1 < c_2 < 1$, $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{d} \in \mathbb{R}^n$. Find α such that

(Armijo rule)
$$f(\mathbf{x} + \alpha \mathbf{d}) \le f(\mathbf{x}) + \alpha c_1 (\nabla f(\mathbf{x}))^T \mathbf{d},$$

(curvature condition)
$$-(\nabla f(\mathbf{x} + \alpha \mathbf{d}))^T \mathbf{d} \leq -c_2(\nabla f(\mathbf{x}))^T \mathbf{d}$$
.

Theorem 12.20. (Wolfe's conditions are not void) Let $f \in C^1(\mathbb{R}^n)$ with $\inf f > -\infty$ and $\mathbf{d} \in \mathbb{R}^n$ be a descent direction at \mathbf{x} . Let $0 < c_1 < c_2 < 1$. Then there exists $\alpha > 0$ with

(Armijo rule)
$$f(\mathbf{x} + \alpha \mathbf{d}) \le f(\mathbf{x}) + \alpha c_1 (\nabla f(\mathbf{x}))^T \mathbf{d},$$
(curvature condition)
$$-(\nabla f(\mathbf{x} + \alpha \mathbf{d}))^T \mathbf{d} \le -c_2 (\nabla f(\mathbf{x}))^T \mathbf{d}.$$

Theorem 12.21. (Strong Wolfe conditions) Let $0 < c_1 < c_2 < \frac{1}{2}$, $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{d} \in \mathbb{R}^n$. Find $\alpha > 0$ such that

$$f(\mathbf{x} + \alpha \mathbf{d}) \le f(\mathbf{x}) + \alpha c_1 \nabla f(\mathbf{x})^T \mathbf{d},$$
$$\left| \nabla f(\mathbf{x} + \alpha \mathbf{d})^T \mathbf{d} \right| \le c_2 \left| \nabla f(\mathbf{x})^T \mathbf{d} \right|.$$

12.2.2 Exact line search

Definition 12.22. 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 **exact line search** method solves the problem

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

Method 12.23. (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 12.24. 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 x satisfies the stop condition.

Definition 12.25. 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

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

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

Remark 12.26. 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 12.27. (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 $\varphi(\lambda) > \varphi(\tilde{\mu})$, 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 12.28. The golden section method is a **linear convergent** method.

Method 12.29. (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 12.30. The Fibonacci method is a linear convergent method.

Method 12.31. (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 $\nabla f(m) \cdot d < 0$, 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 12.32. The bisection method is a linear convergent method.

Method 12.33. (Newton's method) Given the initial point x and $\varepsilon > 0$,

- The iteration step is:

- The solution is **x**.

Theorem 12.34. The Newton's method is a quadratic convergent method.

Unconstrained Optimization

Definition 12.35. 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.

12.3.1 Gradient descent method

Method 12.36. (Gradient descent with exact line search) Given $f \in C^1(\mathbb{R}^n)$,

Initialize: $\mathbf{x}^{[0]} \in \mathbb{R}^n$,

For $k \in \mathbb{N}$,

- (1) Set $\mathbf{d}^{[k]} = -\nabla f(\mathbf{x}^{[k]});$
- (2) Pick $\alpha^{[k]} \in \underset{\alpha \in \mathbb{R}^+}{\arg\min} \{ f(\mathbf{x}^{[k]} + \alpha \mathbf{d}^{[k]}) \};$
- (3) Set $\mathbf{x}^{[k+1]} = \mathbf{x}^{[k]} + \alpha^{[k]} \mathbf{d}^{[k]}$.

Corollary 12.37. (Gradient descent with constant stepsize) Let $f \in C^2(\mathbb{R}^n)$ with $\inf f > 1$ $-\infty$. Suppose that there exists L>0 such that

$$\forall \mathbf{x} \in \mathbb{R}^n, L \ge \|\nabla^2 f(\mathbf{x})\|.$$

For any fixed $\gamma \in (0,2)$, and the sequence generated as

$$x^{[k+1]} = x^{[k]} - \frac{\gamma}{L} \nabla f(x^{[k]}),$$

then any accumulation point of $\{x^{[k]}\}$ is a stationary point of f.

Theorem 12.38. The gradient descent method is a linear convergent method.

12.3.2 Newton's method

Method 12.39. (Newton's method) Given $f \in C^2(\mathbb{R}^n)$,

Initialize: $\mathbf{x}^{[0]} \in \mathbb{R}^n$,

For $k \in \mathbb{N}$,

$$(1) \mathbf{x}^{[k+1]} = \mathbf{x}^{[k]} - \left(\nabla^2 f(\mathbf{x}^{[k]})\right)^{-1} \nabla f(\mathbf{x}^{[k]}).$$

Theorem 12.40. The Newton's method is a quadratic convergent method.

Example 12.41. (Failure of Newton's method) Given function $g = x - x^3$ and starting point $x^{[0]} = \frac{1}{\sqrt{5}}$, then the sequence of iteration is

$$x^{[1]} = -\frac{1}{\sqrt{5}}, x^{[2]} = \frac{1}{\sqrt{5}}, \dots$$

12.3.3 Quasi-Newton methods

Method 12.42. (Secant method) To solve g(x) = 0 where $g(x) \in C^1(\mathbb{R})$. Let $x^{[0]}, x^{[1]} \in \mathbb{R}$ and $g(x^{[0]}) \neq g(x^{[1]})$, for k = 1, ..., use finite difference to approximate g' in Newton's method, i.e.

$$x^{[k+1]} = x^{[k]} - g(x^{[k]}) rac{x^{[k]} - x^{[k-1]}}{g(x^{[k]}) - g(x^{[k-1]})}.$$

Definition 12.43. (Secant equations) Let $f \in C^2(\mathbb{R}^n)$ and given $\mathbf{x}^{[k+1]}$ and $\mathbf{x}^{[k]}$, we expect

$$\nabla^2 f(\mathbf{x}^{[k+1]}) \big(\mathbf{x}^{[k+1]} - \mathbf{x}^{[k]}\big) \approx \nabla f(\mathbf{x}^{[k+1]}) - \nabla f(\mathbf{x}^{[k]}).$$

Let $\mathbf{s}^{[k]} = \mathbf{x}^{[k+1]} - \mathbf{x}^{[k]}$, $\mathbf{y}^{[k]} = \nabla f(\mathbf{x}^{[k+1]}) - \nabla f(\mathbf{x}^{[k]})$ and $B^{[k+1]} = (H^{[k+1]})^{-1}$ be the matrix constructed to approximate $\nabla^2 f(\mathbf{x}^{[k+1]})$,

$$B^{[k+1]}\mathbf{s}^{[k]} = \mathbf{y}^{[k]}, \ H^{[k+1]}\mathbf{y}^{[k]} = \mathbf{s}^{[k]}.$$

Example 12.44. (Popular update formula) Initialize $B^{[0]}$ or $H^{[0]}$ at a positive definite matrix, then update by

DFP:

$$\begin{split} B^{[k+1]} &= \left(I - \frac{\mathbf{y}^{[k]}\mathbf{g}^{[k]}^T}{\mathbf{y}^{[k]^T}\mathbf{s}^{[k]}}\right) B^{[k]} \left(I - \frac{\mathbf{s}^{[k]}\mathbf{y}^{[k]^T}}{\mathbf{y}^{[k]^T}\mathbf{s}^{[k]}}\right) + \frac{\mathbf{y}^{[k]}\mathbf{y}^{[k]}^T}{\mathbf{y}^{[k]^T}\mathbf{s}^{[k]}}, \\ H^{[k+1]} &= H^{[k]} + \frac{\mathbf{s}^{[k]}\mathbf{s}^{[k]}^T}{\mathbf{y}^{[k]^T}\mathbf{s}^{[k]}} - \frac{H^{[k]}\mathbf{y}^{[k]}\mathbf{y}^{[k]}^TH^{[k]}}{\mathbf{y}^{[k]^T}H^{[k]}\mathbf{y}^{[k]}}; \end{split}$$

BFGS:

$$\begin{split} B^{[k+1]} &= B^{[k]} + \frac{\mathbf{y}^{[k]}\mathbf{y}^{[k]^T}}{\mathbf{y}^{[k]^T}\mathbf{s}^{[k]}} - \frac{B^{[k]}\mathbf{s}^{[k]}\mathbf{s}^{[k]^T}B^{[k]}}{\mathbf{s}^{[k]^T}B^{[k]}\mathbf{s}^{[k]}}, \\ H^{[k+1]} &= \bigg(I - \frac{\mathbf{s}^{[k]}\mathbf{y}^{[k]^T}}{\mathbf{y}^{[k]^T}\mathbf{s}^{[k]}}\bigg)H^{[k]}\bigg(I - \frac{\mathbf{y}^{[k]}\mathbf{s}^{[k]^T}}{\mathbf{y}^{[k]^T}\mathbf{s}^{[k]}}\bigg) + \frac{\mathbf{s}^{[k]}\mathbf{s}^{[k]^T}}{\mathbf{y}^{[k]^T}\mathbf{s}^{[k]}}; \end{split}$$

SR1:

$$B^{[k+1]} = B^{[k]} + rac{\left(\mathbf{y}^{[k]} - B^{[k]}\mathbf{s}^{[k]}
ight)\left(\mathbf{y}^{[k]} - B^{[k]}\mathbf{s}^{[k]}
ight)^T}{\left(\mathbf{y}^{[k]} - B^{[k]}\mathbf{s}^{[k]}
ight)^T\mathbf{s}^{[k]}},$$

$$H^{[k+1]} = H^{[k]} + \frac{\left(\mathbf{s}^{[k]} - H^{[k]}\mathbf{y}^{[k]}\right) \left(\mathbf{s}^{[k]} - H^{[k]}\mathbf{y}^{[k]}\right)^T}{\left(\mathbf{s}^{[k]} - H^{[k]}\mathbf{y}^{[k]}\right)^T \mathbf{y}^{[k]}}.$$

Remark 12.45.

- DFP and BFGS are rank-2 updates, while SR1 is rank-1 update.
- Since $B^{[0]}$ and $H^{[0]}$ are symmetric, all $B^{[k]}$ and $H^{[k]}$ are symmetric by induction.
- In practice, BFGS usually performs better.

Method 12.46. (Basic Quasi-Newton method) Given $f \in C^1(\mathbb{R}^n)$,

Initialize: $\mathbf{x}^{[0]} \in \mathbb{R}^n$ and $B^{[0]} \succ 0$ (or $H^{[0]} \succ 0$),

For $k \in \mathbb{N}$,

- (1) Find $\mathbf{d}^{[k]}$ via $B^{[k]}\mathbf{d}^{[k]} = -\nabla f(\mathbf{x}^{[k]})$ (or $\mathbf{d}^{[k]} = -H^{[k]}\nabla f(\mathbf{x}^{[k]})$);
- (2) Update $\mathbf{x}^{[k+1]} = \mathbf{x}^{[k]} + \alpha^{[k]} \mathbf{d}^{[k]}$ where $\alpha^{[k]} > 0$;
- (3) Set $y^{[k]} = \nabla f(\mathbf{x}^{[k+1]}) \nabla f(\mathbf{x}^{[k]})$, $s^{[k]} = \mathbf{x}^{[k+1]} \mathbf{x}^{[k]}$ and compute $B^{[k+1]}$ (or $H^{[k+1]}$).

Proposition 12.47. Let $H^{[k]} \succ 0$ and $\mathbf{y}^{[k]^T} \mathbf{s}^{[k]} > 0$ and $H^{[k+1]}$ be given by BFGS update, then $H^{[k+1]} \succ 0$.

The same conclusion holds if $H^{[k]}$ and $H^{[k+1]}$ are replaced by $B^{[k]}$ and $B^{[k+1]}$, respectively.

Method 12.48. (Quasi-Newton method with Wolfe line search) Given $f \in C^1(\mathbb{R}^n)$ with inf $f > -\infty$,

Initialize: $0 < c_1 < c_2 < 1$, $x^{[0]} \in \mathbb{R}^n$, and $H^{[0]} = \eta I$ for some $\eta > 0$,

For $k \in \mathbb{N}$,

- (1) Find $d^{[k]}$ via $d^{[k]} = -H^{[k]}\nabla f(x^{[k]});$
- (2) Compute $\alpha^{[k]}$ that satisfies the Wolfe's condition;
- (3) Update $x^{[k+1]} = x^{[k]} + \alpha^{[k]}d^{[k]}$;
- $(4) \ \ \mathrm{Set} \ y^{[k]} = \nabla f\big(x^{[k+1]}\big) \nabla f\big(x^{[k]}\big), \ s^{[k]} = x^{[k+1]} x^{[k]} \ \ \mathrm{and} \ \ \mathrm{compute} \ H^{[k+1]} \ \ \mathrm{as} \ \ \mathrm{in} \ \ \mathrm{BFGS}.$

Theorem 12.49. (Zoutendijk's theorem) For $f \in C^1(\mathbb{R}^n)$ with $\inf f > -\infty$, $x^{[0]} \in \mathbb{R}^n$ and exists l > 0 such that for all x, y with $\max\{f(x), f(y)\} \leq f(x^{[0]})$,

$$\|\nabla f(x) - \nabla f(y)\|_2 \leq l\|x-y\|_2.$$

Then for a sequence $\{x^{[k]}\}$ with non-stationary points generated as

$$x^{[k+1]} = x^{[k]} + \alpha^{[k]} d^{[k]},$$

with $d^{[k]}$ a descent direction and $\alpha^{[k]}$ satisfying the Wolfe's condition, then it holds that

$$\sum_{k=0}^{\infty} \cos^2 \left(\theta^{[k]}\right) \left\| \nabla f \left(x^{[k]}\right) \right\|_2^2 < \infty,$$

where

$$\cos(\theta^{[k]}) = \frac{-\left(\nabla f(x^{[k]})\right)^T d^{[k]}}{\left\|\nabla f(x^{[k]})\right\|_2 \left\|d^{[k]}\right\|_2}.$$

Corollary 12.50. If there exists k > 0 such that $\cos(\theta^{[k]}) \ge \delta$ for all k, then $\lim_{k \to \infty} \|\nabla f(x^{[k]})\|_2 = 0$. Hence, any accumulation point of $\{x^{[k]}\}$ is stationary.

For BFGS, if there exists M>0 such that for all $k\in\mathbb{N}$ $\left\|H^{[k]}\right\|_2\left\|\left(H^{[k]}\right)^{-1}\right\|_2< M$, then $\lim_{k\to\infty}\left\|\nabla f\left(x^{[k]}\right)\right\|_2=0$.

Theorem 12.51. The Quasi-Newton method is a superlinear convergent method.

12.4 Linear Programming

Theorem 12.52. (Strong duality for LP, version I) Let $A \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^m$ and $\mathbf{c} \in \mathbb{R}^n$. Consider

$$v_p = \sup_{\mathbf{x} \in \mathbb{R}^n} \big\{ \mathbf{c}^T \mathbf{x} : A\mathbf{x} = \mathbf{b}, \ \mathbf{x} \geq 0 \big\}, v_d = \inf_{\mathbf{y} \in \mathbb{R}^m} \big\{ \mathbf{b}^T \mathbf{y} : \mathbf{c} \leq A^T \mathbf{y} \big\}.$$

Suppose that there exists $\hat{\mathbf{x}} \geq 0$ with $A\hat{\mathbf{x}} = \mathbf{b}$. Then $v_p = v_d$.

Theorem 12.53. (Strong duality for LP, version I) Let $A \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^m$ and $\mathbf{c} \in \mathbb{R}^n$. Consider

$$v_p = \sup_{\mathbf{x} \in \mathbb{R}^n} \big\{ \mathbf{c}^T \mathbf{x} : A\mathbf{x} = \mathbf{b}, \ \mathbf{x} \geq 0 \big\}, v_d = \inf_{\mathbf{y} \in \mathbb{R}^m} \big\{ \mathbf{b}^T \mathbf{y} : \mathbf{c} \leq A^T \mathbf{y} \big\}.$$

Suppose that either

- there exists $\hat{\mathbf{x}} \geq 0$ with $A\hat{\mathbf{x}} = b$; or
- there exists $\hat{\mathbf{y}}$ with $\mathbf{c} \leq A^T \hat{\mathbf{y}}$.

Then $v_p = v_d$ and both optimal values are attained when finite.

Remark 12.54. Recipe for writing dual problems:

	$\max \mathbf{c}^T \mathbf{x}$ s.t. $A \mathbf{x} \mathbf{b}$ $\mathbf{x} \diamondsuit$	$\min \mathbf{b}^T \mathbf{y}$ s.t. $A^T \mathbf{y} \diamondsuit c$ $\mathbf{y} \clubsuit$
*	i -th constraint \leq i -th constraint \geq i -th constraint $=$	i -th variable ≥ 0 i -th variable ≤ 0 i-th variable unrestricted
\langle	j -th variable ≥ 0 j -th variable ≤ 0 j -th variable unrestricted	j -th constraint \geq j -th constraint \leq j -th constraint $=$

12.5 Semidefinite Programming

Definition 12.55. The **primal-dual SDP pairs** is defined as:

Primal	$ \left \begin{array}{l} \displaystyle \min_{X \in S^n} \mathrm{tr}(CX), \\ \mathrm{s.t.} \ \mathrm{tr}(A_iX) = b_i, i = 1,, m \end{array} \right $	
	$X \succeq 0$	
Dual	$egin{aligned} & \max_{\mathbf{y} \in \mathbb{R}^n} \mathbf{b}^T \mathbf{y}, \\ & ext{s.t.} & C - \sum_{i=1}^m \mathbf{y}_i A_i \succeq 0 \end{aligned}$	

where $A_i, C \in S^n$ for all i. Let v_p and v_d denote their optimal values.

Theorem 12.56. (Strong duality for SDPs) Consider the primal-dual SDP pairs, then the following statements holds:

- If there exists $\overline{X} \succ 0$ such that $\operatorname{tr}(A_i \overline{X}) = \mathbf{b}_i$ for all i, then $v_p = v_d$ and v_d is attained while finite.
- If there exists $\overline{\mathbf{y}} \in \mathbb{R}^m$ such that $C \sum_{i=1}^m \overline{\mathbf{y}}_i A_i \succeq 0$, then $v_p = v_d$ and v_p is attained while finite.

Remark 12.57. It always holds that $v_p \ge v_d$, indeed, for any primal feasible X and dual feasible y, we have

$$\mathbf{b}^T y = \sum_{i=1}^m \mathbf{b}_i \mathbf{y}_i = \sum_{i=1}^m \mathrm{tr}(A_i X) \mathbf{y}_i = \mathrm{tr}\left(\sum_{i=1}^m \mathbf{y}_i A_i X\right) = \mathrm{tr}\left(\left(\sum_{i=1}^m \mathbf{y}_i A_i - C\right) X\right) + \mathrm{tr}(CX).$$

Theorem 12.58. Let $A, C \in S_+^n$, then $tr(AC) \ge 0$.

Proposition 12.59. Consider the primal-dual SDP pairs and the set

$$\hat{\Upsilon} = \left\{ \left[\operatorname{tr}(CX), \operatorname{tr}(A_1X), ..., \operatorname{tr}(A_mX) \right]^T \in \mathbb{R}^{m+1} : X \succ 0 \right\}$$

on the previous slide. Suppose that there exists $\overline{y} \in \mathbb{R}^m$ such that $C - \sum_{i=1}^m \overline{y}_i A_i \succ 0$. Then $\hat{\gamma}$ is closed.

Theorem 12.60. (Schur complement) Let $A \in S^m$, $C \in S^n$, $B \in \mathbb{R}^{m \times n}$ and $A \succ 0$, then

$$\begin{pmatrix} A & B \\ B^T & C \end{pmatrix} \succeq 0 \Leftrightarrow C - B^T A^{-1} B \succeq 0.$$

We call $C - B^T A^{-1} B$ the Schur complement of A in $\begin{pmatrix} A & B \\ B^T & C \end{pmatrix}$.

12.6 Penalty/Barrier Methods

Definition 12.61. (Penalty functions) A function $P : \mathbb{R}^n \to \mathbb{R}$ is a penalty function for the constraint set $\{x : \forall i \in I, g_i(\mathbf{x}) \leq 0\}$ if

- $\forall \mathbf{x} \in \mathbb{R}^n, P(\mathbf{x}) \geq 0;$
- $P(\mathbf{x}) = 0$ iff $\forall i \in I, g_i(\mathbf{x}) \leq 0$.

Method 12.62. (Penalty method: basic version) Let c > 0 and $\eta > 1$.

Initialize:
$$\mathbf{x}^{[0]} \in \mathbb{R}^n$$
, $c_1 = c$,

For $k \in \mathbb{N}$,

- (1) Find a minimizer $\mathbf{x}^{[k]}$ of $q_{c_k}(\mathbf{x}) = f(\mathbf{x}) + \frac{c_k}{2} \sum_{i=1}^m (\max(g_i(\mathbf{x}), 0))^2$, using $\mathbf{x}^{[k-1]}$ as the initial point for the iterative method;
- (2) Update $c_{k+1} = \eta c_k$.

Theorem 12.63. Consider

$$\begin{split} & \min_{\mathbf{x} \in \mathbb{R}^n} \quad f(\mathbf{x}) \\ & \text{s.t.} \quad g_i(x) \leq 0, i \in I = \{1, \cdots, m\}, \\ & \text{where } f, g_i \in C^1, \{x : \forall i \in I, g_i(\mathbf{x}) \leq 0\} \neq \emptyset. \end{split}$$

and suppose that $\inf f > 1$. Let $\{\mathbf{x}^{[k]}\}$ be generated by the basic version penalty method. Then any accumulation point x^* of $\{x^{[k]}\}$ is a globally optimal solution.

Method 12.64. (Penalty method: practical version) Let c > 0 and $\eta > 1$.

Initialize: $\mathbf{x}^{[0]} \in \mathbb{R}^n$, $c_1 = c$,

For $k \in \mathbb{N}$,

- (1) Find an $\mathbf{x}^{[k]}$ such that $\nabla q_{c_k}(\mathbf{x}^{[k]}) \approx 0$, using $\mathbf{x}^{[k-1]}$ as the initial point for the iterative method;
- (2) Update $c_{k+1} = \eta c_k$.

Method 12.65. (Barrier method: basic version) Let $\mu > 0$ and $\eta > 1$.

Initialize:
$$\mathbf{x}^{[0]} \in \mathbb{S}^0$$
, $\mu_1 = \mu$,

For $k \in \mathbb{N}$,

- (1) Find a minimizer $\mathbf{x}^{[x]}$ of $f_{\mu_k}(x) = f(x) \mu_k \sum_{i=1}^m \ln(-g_i(\mathbf{x}))$, using $\mathbf{x}^{[k-1]}$ as the initial point for the iterative method;
- (2) Update $\mu_{k+1} = \frac{\mu_k}{\eta}$.

12.7 Conjugate Gradient Method

Method 12.66. (Conjugate gradient method: Conceptual version)

$$\text{Initialize: } \mathbf{x}^{[0]} \in \mathbb{R}^n, \, \mathbf{d}^{[0]} = -\nabla f \big(\mathbf{x}^{[0]}\big) = \mathbf{b} - A\mathbf{x}^{[0]},$$

For $k \in \mathbb{N}$,

- (1) If $d^{[k]} = 0$, terminate;
- $(2) \ \text{Pick} \ \alpha_k \ \text{so that} \ \alpha_k \in \underset{\alpha > 0}{\arg\max} \big\{ f \big(\mathbf{x}^{[k]} + \alpha \mathbf{d}^{[k]} \big) \big\};$

(3) Set
$$\mathbf{x}^{[k+1]} = \mathbf{x}^{[k]} + \alpha_k \mathbf{d}^{[k]}$$
 and $d^{[k+1]} = -\nabla f(\mathbf{x}^{[k+1]}) - \sum_{i=0}^k \frac{-\nabla f(\mathbf{x}^{[k+1]})^T A \mathbf{d}^{[j]}}{\mathbf{d}^{[j]}^T A \mathbf{d}^{[j]}} \mathbf{d}^{[j]}$.

Theorem 12.67. Let $A \succ 0$ and $\mathbf{x}^{[0]} \in \mathbb{R}^n$. Set $d^{[0]} = -\nabla f(\mathbf{x}^{[0]})$. For $k \in \mathbb{N}$, suppose that $\mathbf{d}^{[0]}, ..., \mathbf{d}^{[k]} \neq 0$, where for each i = 0, ..., k - 1,

$$\mathbf{d}^{[i+1]} = -\nabla f(\mathbf{x}^{[i+1]}) - \sum_{i=0}^{i} \frac{-\nabla f(\mathbf{x}^{[i+1]})^{T} A \mathbf{d}^{[j]}}{\mathbf{d}^{[j]^{T}} A \mathbf{d}^{[j]}} \mathbf{d}^{[j]},$$

with $\mathbf{x}^{[i+1]} = \mathbf{x}^{[i]} + \alpha_i \mathbf{d}^{[i]}$ and α_i coming from exact line search. Then for j < k+1, $\nabla f(\mathbf{x}^{[j]})^T \nabla f(\mathbf{x}^{[k+1]}) = 0$ and $\mathbf{d}^{[j]T} \nabla f(\mathbf{x}^{[k+1]}) = 0$.

Theorem 12.68. For $k \in \mathbb{N}$, $\mathbf{x}^{[k]}$, $\mathbf{d}^{[k]}$ are generated by conjugate gradient method, then

$$\mathbf{d}^{[k+1]} = -\nabla f \left(\mathbf{x}^{[k+1]}\right) + \frac{\left\|\nabla f \left(\mathbf{x}^{[k+1]}\right)\right\|_2^2}{\left\|\nabla f \left(\mathbf{x}^{[k]}\right)\right\|_2^2} \mathbf{d}^{[k]}.$$

Method 12.69. (Conjugate gradient method: Formal version)

 $\text{Initialize: } \mathbf{x}^{[0]} \in \mathbb{R}^n, \, \mathbf{d}^{[0]} = -\nabla f \big(\mathbf{x}^{[0]}\big) = \mathbf{b} - A\mathbf{x}^{[0]},$

For $k \in \mathbb{N}$,

- (1) If $d^{[k]} = 0$, terminate;
- (2) Pick α_k so that $\alpha_k \in \underset{\alpha>0}{\operatorname{arg\,max}} \{ f(\mathbf{x}^{[k]} + \alpha \mathbf{d}^{[k]}) \};$

(3) Set
$$\mathbf{x}^{[k+1]} = \mathbf{x}^{[k]} + \alpha_k \mathbf{d}^{[k]}$$
 and $\mathbf{d}^{[k+1]} = -\nabla f(\mathbf{x}^{[k+1]}) + \frac{\|\nabla f(\mathbf{x}^{[k+1]})\|_2^2}{\|\nabla f(\mathbf{x}^{[k]})\|_2^2} \mathbf{d}^{[k]}$.

Method 12.70. (Conjugate gradient method: Actual version)

Initialize: $\mathbf{x}^{[0]} \in \mathbb{R}^n$, $\mathbf{r}^{[0]} = \mathbf{d}^{[0]} = -\nabla f(\mathbf{x}^{[0]}) = \mathbf{b} - A\mathbf{x}^{[0]}$,

For $k \in \mathbb{N}$,

- (1) If $||r^{[k]}||$ (or less commonly, $||d^{[k]}||$) is below a tolerance, terminate;
- $(2) \ \text{Compute } \alpha_k = \frac{\mathbf{r}^{[k]^T}\mathbf{r}^{[k]}}{\mathbf{d}^{[k]^T}A\mathbf{d}^{[k]}}, \, \mathbf{x}^{[k+1]} = \mathbf{x}^{[k]} + \alpha_k\mathbf{d}^{[k]}, \, \mathbf{r}^{[k+1]} = \mathbf{r}^{[k]} \alpha_kA\mathbf{d}^{[k]};$
- (3) Compute $\beta_k = \frac{\mathbf{r}^{[k+1]^T}\mathbf{r}^{[k+1]}}{\mathbf{r}^{[k]^T}\mathbf{r}^{[k]}}, \mathbf{d}^{[k+1]} = \mathbf{r}^{[k+1]} + \beta_k \mathbf{d}^{[k]}.$

Theorem 12.71. (Luenberger) Consider the conjugate gradient method for minimizing $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A \mathbf{x} - \mathbf{b}^T \mathbf{x}$ for some $\mathbf{b} \in \mathbb{R}^n$ and $A \succ 0$. Let $\{\mathbf{x}^{[k]}\}$ be the sequence generated and let \mathbf{x}^* be the minimizer of f. If A has eigenvalues $0 < \lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$, then

$$\lambda_1 \big\| \mathbf{x}^{[k+1]} - \mathbf{x}^* \big\|_2^2 \leq \big(\mathbf{x}^{[k+1]} - \mathbf{x}^* \big)^T A \big(\mathbf{x}^{[k+1]} - \mathbf{x}^* \big) \leq \bigg(\frac{\lambda_{n-k} - \lambda_1}{\lambda_{n-k} + \lambda_1} \bigg)^2 \big(\mathbf{x}^{[0]} - \mathbf{x}^* \big)^T A \big(\mathbf{x}^{[0]} - \mathbf{x}^* \big)$$

Method 12.72. (Nonlinear conjugate gradient method: Conceptual version)

Initialize: $\mathbf{x}^{[0]} \in \mathbb{R}^n$, $\mathbf{d}^{[0]} = -\nabla f(\mathbf{x}^{[0]})$,

For $k \in \mathbb{N}$,

- (1) If $d^{[k]}$ is small, terminate;
- (2) Pick α_k judiciously (e.g. exact line search, strong Wolfe conditions);

(3) Set
$$\mathbf{x}^{[k+1]} = \mathbf{x}^{[k]} + \alpha_k \mathbf{d}^{[k]}$$
 and $\mathbf{d}^{[k+1]} = -\nabla f(\mathbf{x}^{[k+1]}) + \frac{\|\nabla f(\mathbf{x}^{[k+1]})\|_2^2}{\|\nabla f(\mathbf{x}^{[k]})\|_2^2} \mathbf{d}^{[k]}$.

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

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

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

$$\forall i = 1, 2, ..., s, \quad \mathbf{p}(t_n) = \mathbf{u}_n \text{ and } \mathbf{p}'(t_n + c_i k) = \mathbf{f}(\mathbf{p}(t_n + c_i k), t_n + c_i k),$$

(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

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

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

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

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 $f(\mathbf{u}, t)$ Lipschitz continuous in \mathbf{u} and continuous in t yields

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

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

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

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

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

13.4.3 Trapezoidal method

Definition 13.33. The **trapezoidal method** solves the IVP by

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

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

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

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

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

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

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

Finite Element Method

Definition 14.1. A function $a(\cdot, \cdot)$ is a **bilinear function** if for all $u, v \in V$, $k_1, k_2 \in F$,

- $a(k_1u + k_2v, w) = k_1a(u, w) + k_2a(v, w),$
- $a(u, k_1v + k_2w) = k_1a(u, v) + k_2a(u, w)$.

A bilinear function is **bounded** or **continuous** if $\|\cdot\|$ is the norm on V, and for all $u, v \in V$, exists M > 0, such that

$$|a(u,v)| \le M||u|||v||.$$

A bilinear function is **symmetric** if for all $u, v \in V$, a(u, v) = a(v, u).

A bilinear function is **V-elliptic** if exists $\alpha > 0$, for all $v \in V$,

$$\alpha \|v\|^2 \le a(v, v).$$

Definition 14.2. Given a normed linear space V with a bounded bilinear function $a(\cdot, \cdot)$ on it and $f \in V^*$, then for $U \subset V$,

$$J(u)=\inf_{v\in U}J(v), J(v)=\frac{1}{2}a(v,v)-f(v).$$

Theorem 14.3. The solution to problem 14.2. exists and unique if

- V is complete,
- U is a closed convex subset of V,
- $a(\cdot, \cdot)$ is symmetric and V-elliptic.

Theorem 14.5. If u is the solution to problem 14.2., if and only if

$$\forall v \in U, a(u, v - u) \ge f(v - u).$$

where a(u, u) = f(u) if U is a convex cone with the apex $\mathbf{0}$, $\forall v \in U, a(u, v) = f(v)$ if U is a closed subset of V.

Theorem 14.7. (Lax-Milgram lemma) Given a Hilbert space V, $a(\cdot, \cdot): V \times V \to \mathbb{R}$ is a continuous V-elliptic bilinear function, $f: V \to \mathbb{R}$ a continuous linear functional, then there exists only $u \in V$, such that

$$\forall v \in V, a(u, v) = f(v).$$

Lemma 14.8. Given $u \in H_0^2(\Omega)$, $|\cdot|$ is the Sobolev seminorm, $||\cdot||$ is the Sobolev norm, then

$$\|\Delta u\|_{0,\Omega}^2 = |u|_{2,\Omega}^2$$
.

Theorem 14.9. (Poincare-Friedrichs) Given a bounded set Ω , $v \in H_0^m(\Omega)$, then there exists a constant $C(\Omega)$, such that

$$||v||_{0,\Omega} \leq C(\Omega)|v|_{m,\Omega}.$$

14.1 Galerkin Method

Notation 14.10. $V_h \subset V$ denotes a given finite dimensional subspace.

Definition 14.11. The idea of Galerkin method is to solve the $u_h \in V_h$, such that

$$a(u_h, v_h) = f(v_h).$$

Definition 14.12. The idea of Ritz method is to solve the $u_h \in V_h$, such that

$$J(u_h) = \min_{v_h \in V_h} J(v_h),$$

where

$$J(v) = \frac{1}{2}a(v,v) - f(v).$$

Definition 14.13. A k-simplex is a k-dimensional convex hull of k+1 vertices. Given $x_0, ..., x_n \in \mathbb{R}^n$ affinely independent vectors, then a n-simplex is defined as

$$K_n = \Bigg\{ \sum_{i=1}^n \theta_i x_i : \sum_{i=1}^n \theta_i = 1, \forall j \in [0,n] \cap \mathbb{Z}, \theta_j \geq 0 \Bigg\}.$$

Definition 14.14. Let $\dim(V_h) = N$ and $\varphi_1, ..., \varphi_N$ be the basis functions of V_N , then the matrix $K = (a(\varphi_i, \varphi_j))_{N \times N}$ is the **stiffness matrix**, and $F = (f(\varphi_i))_N$ is the **load vector**.

Theorem 14.15. Let $a(\cdot, \cdot): V \times V \to \mathbb{R}^n$ be a bilinear symmetric V-elliptic function, then the corresponding stiffness matrix is symmetric and positive definite.

Number Theory

15.1 Prime Number

Definition 15.1. A **prime number** (or a **prime**) is a natural number greater than 1 that is not a product of two smaller natural numbers.

Definition 15.2. A **composite number** (or a **composite**) is a natural number greater than 1 that is a product of two smaller natural numbers.

15.1.1 Primality testing

Theorem 15.3. For a integer $n \in \mathbb{N}$, if it is a product of two natural number a and b that $a \leq b$, then

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

Method 15.4. (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 15.5. (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 15.6. 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.

15.1.2 Sieves

Method 15.7. (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;

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(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

16.1 Linear Regression

Definition 16.1. 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 16.2. 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 17 Decision Tree

Chapter 18 Support Vector Machine

Cluster

19.1 K-means

Definition 19.1. 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 19.2. 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,

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

Method 19.3. (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 20 Neural Networks