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1 Review

1.1 Calculus

Definition 1.1 – Norm

$\|\cdot\| : \mathbb{R}^n \rightarrow \mathbb{R}$ is a mapping from \mathbb{R}^n to \mathbb{R} such that

- For every $\mathbf{x} \in \mathbb{R}^n$, $\|\mathbf{x}\| \geq 0$
- $\|\mathbf{x}\| = 0$ if and only if $\mathbf{x} = \mathbf{0}$.
- For every $\alpha \in \mathbb{R}$ and for every $\mathbf{x} \in \mathbb{R}^n$, $\|\alpha\mathbf{x}\| = |\alpha|\|\mathbf{x}\|$
- (Triangle inequality) For every $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$,

$$\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$$

Two common norms, ℓ_1 and ℓ_2 norms:

1. ℓ_1 : $\|\mathbf{x}\|_1 = \sum_{i=1}^n |x_i| = |x_1| + |x_2| + \cdots + |x_n|$
2. ℓ_2 : $\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^n x_i^2} = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}$

Proposition 1.1 – Cauchy-Schwarz Inequality

For every $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$

$$|\mathbf{x}^T \mathbf{y}| = \langle \mathbf{x}, \mathbf{y} \rangle \leq \|\mathbf{x}\|_2 \|\mathbf{y}\|_2$$

with equality if and only if $\mathbf{x} = \alpha \mathbf{y}$ for some $\alpha \in \mathbb{R}$.

Definition 1.2 – Neighborhood/Open ball

Given $\delta > 0$, $\bar{\mathbf{x}} \in \mathbb{R}^n$, the open ball $B_\delta(\bar{\mathbf{x}}) = \{\mathbf{x} \in \mathbb{R}^n \mid \|\mathbf{x} - \bar{\mathbf{x}}\|_2 < \delta\}$

Definition 1.3 – Sequence Convergence in \mathbb{R}^n

We say that a sequence $\{\mathbf{x}_k\} \subseteq \mathbb{R}^n$ converges to $\mathbf{x}^* \in \mathbb{R}^n$ and write

$$\lim_{k \rightarrow \infty} \mathbf{x}_k = \mathbf{x}^*$$

if for every $\epsilon > 0$ there exists $N \in \mathbb{N}$ such that for every $k \geq N$, $\|\mathbf{x}_k - \mathbf{x}^*\| < \epsilon$.

Definition 1.4 – Limit Point

If $\{\mathbf{x}_k\}$ has a subsequence that converges to \mathbf{x}^* , then \mathbf{x}^* is called a limit point of $\{\mathbf{x}_k\}$.

Given a set $E \subseteq \mathbb{R}^n$, if there exists a sequence $\{\mathbf{x}_k\} \subseteq E$ that converges to \mathbf{x}^* , then \mathbf{x}^* is called a limit point of E .

Definition 1.5 – Closed Set

A set $E \subseteq \mathbb{R}^n$ is closed if it contains all of its limit points.

That is, for every sequence $\{\mathbf{x}_k\} \subseteq E$ with

$$\lim_{k \rightarrow \infty} \mathbf{x}_k = \mathbf{x}^*$$

if $\mathbf{x}^* \in E$, then E is closed.

Definition 1.6 – Interior Point

A point $\mathbf{x} \in E$ is an interior point of E if there is a neighborhood/open ball of \mathbf{x} that is contained in E .

Definition 1.7 – Open Set

A set E is open if all of its elements are interior points.

So, for any point you pick in E , you can find a small neighborhood around that point which is entirely contained in E (there are no boundary points in E).

Theorem 1.1 – Properties of Open/Closed Sets

The followings hold:

- A set is closed (open) if its complement, $\mathbb{R}^n \setminus E$, is open (closed).
- Union of finitely many closed sets is closed
- Intersection of (finitely or infinitely many) closed sets is closed.
- Intersection of finitely many open sets is open
- Union of (finitely or infinitely many) open sets is open.

Definition 1.8 – Bounded

A set $E \subset \mathbb{R}^n$ is bounded if it can be contained in a ball of finite radius. That is, there exists a neighborhood, $B_\delta(\mathbf{x})$, such that $E \subseteq B_\delta(\mathbf{x})$.

Definition 1.9 – Compact

A set $E \subset \mathbb{R}^n$ is compact if it is closed and bounded.

Definition 1.10 – Lipschitz Continuous/Contraction

Let $E \subseteq \mathbb{R}^n$. Let $f : E \rightarrow \mathbb{R}^m$ be a function. We say f is Lipschitz continuous on E if there exists a constant $L > 0$ such that for all $\mathbf{x}, \mathbf{y} \in E$,

$$\|f(\mathbf{x}) - f(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\|$$

Theorem 1.2 – Continuity of Functions

Let $E \subseteq \mathbb{R}^n$, $f, g : E \rightarrow \mathbb{R}^m$ and $\alpha \in \mathbb{R}$. If f and g are continuous at \mathbf{x}_0 , then

1. $f + g, fg, \alpha f$ are continuous at \mathbf{x}_0
2. $\frac{f}{g}$ is continuous at \mathbf{x}_0 provided that $g(\mathbf{x}_0) \neq 0$.

Definition 1.11 – Formal Definition of Derivative

The **derivative** of f at a is defined as

$$f'(a) = \lim_{x \rightarrow a} \frac{f(x) - f(a)}{x - a}$$

if the limit exists.

An alternate definition is

$$f'(a) = \lim_{h \rightarrow 0} \frac{f(a+h) - f(a)}{h}$$

Theorem 1.3 – Extreme Value Theorem (EVT)

If $E \subset \mathbb{R}^n$ is a compact set (closed and bounded) and $f : E \rightarrow \mathbb{R}$ is a continuous function, then f attains a maximum and minimum on E . That is, there exists points $\mathbf{x}_{\min}, \mathbf{x}_{\max} \in E$ such that for all $\mathbf{x} \in E$,

$$f(x) \leq f(\mathbf{x}_{\max}) \quad \text{and} \quad f(\mathbf{x}_{\min}) \leq f(\mathbf{x})$$

Theorem 1.4 – Continuously Differentiable

f is continuously differentiable at \mathbf{x}_0 if all partial derivatives exist and are continuous in a neighborhood of \mathbf{x}_0 . We say f is continuously differentiable, $f \in C^1$, if its partial derivatives are continuous everywhere.

f is twice differentiable on E if $\nabla^2 f(x)$ exists for all $\mathbf{x} \in E$. If each entry of the Hessian $\nabla^2 f(\mathbf{x})$ is continuous, we say f is twice differentiable on E , $f \in C^2$.

Theorem 1.5

If $f : E \rightarrow \mathbb{R}$ is twice differentiable, then the Hessian is symmetric.

Theorem 1.6 – Mean Value Theorem (MVT)

Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be continuous on the closed interval $[a, b]$ and differentiable on the open interval (a, b) . Then there exists $c \in (a, b)$ such that

$$f(b) - f(a) = f'(c)(b - a)$$

Lemma 1.1 – Directional Derivative

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $\bar{x}, d \in \mathbb{R}^n$ where d is the direction. We define

$$\phi(\epsilon) = f(\bar{x} + \epsilon d) : \mathbb{R} \rightarrow \mathbb{R}$$

the value of the function f at a point that is displaced from \bar{x} by a distance of ϵ in the direction d . Then the **directional derivative**, denoted $f'(x; d)$ of f at x at the direction d is

$$f'(x; d) = \phi'(0) = \lim_{\epsilon \rightarrow 0} \frac{f(x + \epsilon d) - f(x)}{\epsilon} = \nabla f(x)^T d$$

Definition 1.12 – Directional Derivative (Different notation)

The directional derivative of f at a point $\bar{x} \in \mathbb{R}^n$ in the direction d is

$$f'(\bar{x}; d) = \left. \frac{d}{ds} f(\bar{x} + sd) \right|_{s=0}$$

Theorem 1.7

If f is differentiable at \bar{x} , then

$$f'(\bar{x}; d) = \nabla f(\bar{x})^T d$$

Proof. We only prove in the case where $\bar{x} = (a, b) \in \mathbb{R}^2$.

$$\begin{aligned}
 f'(\bar{x}; d) &= \left. \frac{d}{ds} f(\bar{x} + sd) \right|_{s=0} \\
 &= \left. \frac{d}{ds} f(\underbrace{a + sd_1}_x, \underbrace{b + sd_2}_y) \right|_{s=0} \\
 &= \left[\frac{\partial f}{\partial x} \frac{dx}{ds} + \frac{\partial f}{\partial y} \frac{dy}{ds} \right]_{s=0} && \text{Chain rule} \\
 &= \left[\frac{\partial}{\partial x} f(a + sd_1, b + sd_2) \cdot d_1 + \frac{\partial}{\partial y} f(a + sd_1, b + sd_2) \cdot d_2 \right]_{s=0} \\
 &= \frac{\partial f}{\partial x}(a, b) \cdot d_1 + \frac{\partial f}{\partial y}(a, b) \cdot d_2 \\
 &= \left(\frac{\partial f}{\partial x}(a, b), \frac{\partial f}{\partial y}(a, b) \right) \cdot (d_1, d_2) \\
 &= \nabla f(a, b) \cdot d
 \end{aligned}$$

□

Problem 1.1

Let $f(x, y, z) = x^2z + y^3z^2 - xyz$ with $d = \begin{pmatrix} -1 \\ 0 \\ 3 \end{pmatrix}$. Then the **directional derivative** in the direction d is

$$\nabla f(x, y, z)^T d = \begin{pmatrix} 2xz - yz \\ 3y^2z^2 - xz \\ x^2 + 2y^3z - xy \end{pmatrix}^T \begin{pmatrix} -1 \\ 0 \\ 3 \end{pmatrix} = -2xz + yz + 3x^2 + 6y^3z - 3xy$$

Theorem 1.8 – Taylor’s Theorem on the real line

Let $f : (a, b) \rightarrow \mathbb{R}$, and $\bar{x}, x \in (a, b)$. Then the Taylor’s series centered at \bar{x} (approximation near \bar{x}) is

$$f(x) = f(\bar{x}) + f'(\bar{x})(x - \bar{x}) + \frac{f''(z)}{2}(x - \bar{x})^2$$

where z is between x and \bar{x} that gives the largest value of $f''(z)$. The term $\frac{f''(z)}{2}(x - \bar{x})^2$ is the **error term**

Equivalently,

$$f(\bar{x} + \Delta x) = \underbrace{f(x) + f'(x)\Delta x}_{\text{Linear approximation}} + o(|\Delta x|) \text{ (little O)}$$

This formula emphasizes its use in approximating changes in f for small changes in x , denoted Δx . $o(|\Delta x|)$, the error term, means that the error goes to 0 faster than $|\Delta x|$ as Δx goes to 0. Therefore, this is saying that the linear approximation becomes more and more accurate for smaller Δx .

Theorem 1.9 – Multivariate Taylor

Consider a C^2 -smooth function $f : U \rightarrow \mathbb{R}$ on an open set $U \subset \mathbb{R}^n$. If \bar{x} and x are such that the segment $[\bar{x}, x] := \{\bar{x} + t(x - \bar{x}) : t \in [0, 1]\}$ is contained in U , then the Taylor series expansion of f centered

around \bar{x} is

$$f(x) = f(\bar{x}) + \langle \nabla f(\bar{x}), x - \bar{x} \rangle + \frac{1}{2} \langle \nabla^2 f(z)(x - \bar{x}), (x - \bar{x}) \rangle$$

where z is between x and \bar{x} .

Theorem 1.10 – Taylor’s Theorem

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be continuously differentiable and let $\mathbf{d} \in \mathbb{R}^n$ be a direction vector. Then

$$f(\mathbf{x} + \mathbf{d}) = f(\mathbf{x}) + \underbrace{\nabla f(\mathbf{x} + t\mathbf{d})^T \mathbf{d}}_{\text{directional derivative}}$$

for some $t \in (0, 1)$. Moreover, if f is twice differentiable, then

$$f(\mathbf{x} + \mathbf{d}) = f(\mathbf{x}) + \nabla f(\mathbf{x})^T \mathbf{d} + \frac{1}{2} \underbrace{\mathbf{d}^T \nabla^2 f(\mathbf{x} + t\mathbf{d}) \mathbf{d}}_{\text{second order directional derivative}}$$

for some $t \in (0, 1)$.

This theorem provides a way to approximate the value of the function f at a point $\mathbf{x} + \mathbf{d}$ based on the value and derivatives of f at or near the point \mathbf{x} .

Theorem 1.11 – Taylor’s Theorem (alternative)

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be continuously differentiable at \mathbf{x}^* . Then $\forall \mathbf{x} \in \mathbb{R}^n$

$$f(\mathbf{x}) = \underbrace{f(\mathbf{x}^*) + \nabla f(\mathbf{x}^*)^T (\mathbf{x} - \mathbf{x}^*)}_{\text{linear approximation of } f \text{ at } \mathbf{x}^*} + o(\|\mathbf{x} - \mathbf{x}^*\|)$$

where $o(\|\mathbf{x} - \mathbf{x}^*\|)$ is the error term that goes to 0 faster than $\|\mathbf{x} - \mathbf{x}^*\|$ as $\mathbf{x} \rightarrow \mathbf{x}^*$.

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be twice continuously differentiable at \mathbf{x}^* . Then $\forall \mathbf{x} \in \mathbb{R}^n$

$$f(\mathbf{x}) = \underbrace{f(\mathbf{x}^*) + \nabla f(\mathbf{x}^*)^T (\mathbf{x} - \mathbf{x}^*) + \frac{1}{2} (\mathbf{x} - \mathbf{x}^*)^T \nabla^2 f(\mathbf{x}^*) (\mathbf{x} - \mathbf{x}^*)}_{\text{quadratic approximation of } f \text{ at } \mathbf{x}^*} + o(\|\mathbf{x} - \mathbf{x}^*\|^2)$$

where $o(\|\mathbf{x} - \mathbf{x}^*\|^2)$ is the error term that goes to 0 faster than $\|\mathbf{x} - \mathbf{x}^*\|^2$ as $\mathbf{x} \rightarrow \mathbf{x}^*$.

Problem 1.2 – Lagrange Multiplier Example

Maximize $f(x, y) = x^2 y$ subject to $g(x, y) = x^2 + y^2 = 1$. By using Lagrange multipliers, we know that the maximizer, (x^*, y^*) satisfies

$$\nabla f(x^*, y^*) = \lambda \nabla g(x^*, y^*)$$

We have

$$\begin{aligned} \nabla g(x, y) &= \begin{bmatrix} 2x \\ 2y \end{bmatrix} \\ \nabla f(x, y) &= \begin{bmatrix} 2xy \\ x^2 \end{bmatrix} \end{aligned}$$

Then, using Lagrange multipliers, we solve

$$\begin{bmatrix} 2xy \\ x^2 \end{bmatrix} = \lambda \begin{bmatrix} 2x \\ 2y \end{bmatrix}$$

Since we also have the constraint $x^2 + y^2 = 1$, we solve the system of equations

$$\begin{aligned} 2xy &= 2\lambda x \\ x^2 &= 2\lambda y \\ x^2 + y^2 &= 1 \end{aligned}$$

Solving it, we get

$$(x, y) = \left(\pm\sqrt{\frac{2}{3}}, \pm\sqrt{\frac{1}{3}} \right), \quad \lambda = y$$

Testing each point, we get that $\left(\sqrt{\frac{2}{3}}, \sqrt{\frac{1}{3}} \right)$ is the maximizer of f .

1.2 Linear Algebra

Definition 1.13 – Characteristic Polynomial

The characteristic polynomial of $A \in \mathbb{R}^{n \times n}$ is

$$p(\lambda) = \det(A - \lambda I)$$

The degree of $p(\lambda)$ is n , and the leading term is $(-1)^n \lambda^n$.

The eigenvalues of A are the roots of the characteristic polynomial.

Definition 1.14 – Eigenvectors and Eigenvalues

$0 \neq v \in \mathbb{R}^n$ is an **eigenvector** of A if there exists $\lambda \in \mathbb{R}$ such that $Av = \lambda v$. The number λ is called an **eigenvalue** of A .

Theorem 1.12 – Finding Eigenvectors and Eigenvalues

Let A be a matrix.

1. Set up the characteristic equation. We find

$$\det(A - \lambda I) = 0$$

2. Solve for λ . These are the eigenvalues.
3. Plug eigenvalues $\lambda_1, \dots, \lambda_n$ into $(A - \lambda I)v = 0$ and solve for v . These are the eigenvectors.

Definition 1.15 – Quadratic Form

Let A be a symmetric matrix and $x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$. The **quadratic form** Q of the matrix A is defined as

$$Q = x^T A x$$

Problem 1.3 – Example

Consider the matrix $A = \begin{bmatrix} 5 & -5 \\ -5 & 1 \end{bmatrix}$. The quadratic form of A is

$$Q(x) = 5x_1^2 - 10x_1x_2 + x_2^2$$

Definition 1.16 – Classification of Quadratic Forms

Let $Q = x^T A x$ be a quadratic form of a matrix A . Then A is

1. positive definite if $Q(x) > 0$ for all non-zero vectors x , and $Q(x) = 0$ if and only if $x = 0$. Or all eigenvalues of A are positive. Denoted by $A \succ 0$.
2. positive semidefinite if $Q(x) \geq 0$ for all vectors x , with $Q(x) = 0$ occurring for some non-zero vectors x . Or all eigenvalues of A are non-negative. Denoted by $A \succeq 0$.
3. negative definite if $Q(x) < 0$ for all non-zero vectors x , and $Q(x) = 0$ if and only if $x = 0$. Or all eigenvalues of A are negative. Denoted by $A \prec 0$.
4. negative semidefinite if $Q(x) \leq 0$ for all vectors x , with $Q(x) = 0$ occurring for some non-zero vectors x . Or all eigenvalues of A are non-positive. Denoted by $A \preceq 0$.
5. indefinite if $Q(x)$ can be positive or negative. Or there are positive and negative eigenvalues for A .

Theorem 1.13 – Orthogonal Spectral Decomposition

Let $A \in \mathbb{S}^n$. Then A has an **orthogonal spectral decomposition**

$$A = \sum_i \lambda_i u_i u_i^T = U D U^T$$

where U is orthogonal with the orthogonal eigenvectors u_i as columns and D is a diagonal matrix with real eigenvalues on the diagonal.

Proposition 1.2

Let $A \in \mathbb{S}^n$. The following are equivalent (Positive definite):

1. $A \succ 0$.
2. All the eigenvalues of A are in \mathbb{R}_{++}^n , the interior of the nonnegative orthant.
3. A has a real symmetric positive definite square root, $A = S S$, $S \in \mathbb{S}_{++}^n$.
4. A has a lower triangular factorization, a Cholesky factorization, $A = L L^T$ and L has positive diagonal elements.
5. All principal minors of A are positive.
6. All leading principal minors of A are positive.

And the following are equivalent (Positive semidefinite):

1. $A \succeq 0$.
2. All the eigenvalues of A are in \mathbb{R}_+^n , the nonnegative orthant.
3. A has a real symmetric square root, $A = S S$, $S \in \mathbb{S}^n$.

4. A has a lower triangular factorization, a Cholesky factorization, $A = LL^T$.
5. All principal minors of A are nonnegative.

Definition 1.17 – Principal Submatrices

Let

$$A = \begin{bmatrix} 1 & 1 & 2 & 7 \\ 1 & 1 & 4 & 6 \\ 2 & 4 & 7 & 8 \\ 7 & 6 & 8 & 1 \end{bmatrix}, \quad I = \{1, 3\}, \quad A[I] = \begin{bmatrix} 1 & 2 \\ 2 & 7 \end{bmatrix}$$

Then $A[I]$ is a **principal submatrix** of A .

Definition 1.18 – Principal Minors

Let $A \in \mathbb{S}^n$, where \mathbb{S}^n is the set of all symmetric $n \times n$ matrices.

1. $\det(A[I])$ is called the **principal minor** of A .
2. If $I = \{1, \dots, k\}$ then $\det(A[I])$ is called the **leading principal minor** of A .

Proposition 1.3 – Characterizing Positive Definiteness with Principal Minors

Let $A \in \mathbb{S}^n$. Then

1. $A \succeq 0 \iff \det(A[I]) \geq 0$ for all principal minors $\det(A[I])$.
2. $A \succ 0 \iff \det(A[I]) > 0$ for all **leading** principal minors $\det(A[I])$.

Theorem 1.14

Let $A \in \mathbb{R}^{n \times n}$ be symmetric. Then the following are equivalent:

1. A is positive semidefinite (definite).
2. All eigenvalues of A are nonnegative (positive).
3. A can be factored as $A = BB^T$ where B is an $n \times p$ matrix for some p . (Cholesky factorization)

Definition 1.19 – Diagonally Dominant

A matrix A is diagonally dominant if for every i ,

$$|a_{ii}| \geq \sum_{j \neq i} |a_{ij}|$$

So each diagonal element is greater than or equal to the sum of the absolute values of the other elements in the same row.

It is called strictly diagonally dominant if for every i ,

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}|$$

Proposition 1.4

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric, diagonally dominant matrix whose diagonal entries are nonnegative, then A is positive semidefinite.

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric, strictly diagonally dominant matrix whose diagonal entries are positive, then A is positive definite.

Note that the converse is not true.

Definition 1.20 – Four Fundamental Subspaces

Let A be a $m \times n$ matrix.

- The range space of A is defined as $\text{Range}(A) = \{Ax : x \in \mathbb{R}^n\} \subseteq \mathbb{R}^m$.
- The range space of A^T is defined as $\text{Range}(A^T) = \{A^T y : y \in \mathbb{R}^m\} \subseteq \mathbb{R}^n$.
- The null space of A is defined as $\text{Null}(A) = \{x \in \mathbb{R}^n : Ax = 0\} \subseteq \mathbb{R}^n$.
- The null space of A^T is defined as $\text{Null}(A^T) = \{y \in \mathbb{R}^m : A^T y = 0\} \subseteq \mathbb{R}^m$.

Theorem 1.15 – Rank Nullity Theorem

Let A be an $m \times n$ matrix. Then

$$\text{rank}(A) + \dim(\text{Null}(A)) = n$$

Recall that rank of a matrix is the number of pivots in the reduced row echelon form of the matrix. The dimension of a subspace is the number of linearly independent vectors that span the subspace.

2 Introduction

2.1 Lecture 1-Preliminaries

Definition 2.1 – Big O and little o

Big O is basically the rate of growth of that function. A function $f(n)$ is of order 1, or $O(1)$ if there exists some non zero constant c such that

$$\frac{f(n)}{c} \rightarrow 1$$

as $n \rightarrow \infty$.

Little o is the upper bound of the rate of growth of that function. Therefore, a function $f(n)$ is of order 1, or $o(1)$ if for all constants $c > 0$,

$$\frac{f(n)}{c} \rightarrow 0$$

as $n \rightarrow \infty$.

Definition 2.2 – Differentiability Based on Big o and Little o

If f is differentiable at $x = a$, then

$$f(a + h) = f(a) + f'(a)h + o(h)$$

Conversely, if there exists constants A and B such that

$$f(a + h) = A + Bh + o(h)$$

then f is differentiable at $x = a$. Moreover, $A = f(a)$ and $B = f'(a)$.

Definition 2.3 – Product Rule

If f, g are differentiable at $x = a$, then

$$f(a + h) = f(a) + f'(a)h + o(h), \quad g(a + h) = g(a) + g'(a)h + o(h)$$

Then

$$\begin{aligned} p(a + h) &= f(a + h)g(a + h) \\ &= f(a)g(a) + [f(a)g'(a) + g(a)f'(a)]h + o(h) \end{aligned}$$

Then by above theorem, $p = fg$ is differentiable at $x = a$, and $p'(a) = f(a)g'(a) + g(a)f'(a)$.

Definition 2.4 – Chain Rule

WIP

Definition 2.5 – Inner Product Space

Let $x \in \mathbb{R}^n$, represented as:

$$x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

The inner product space is defined as:

$$\langle x, y \rangle = x^T y = \sum_{i=1}^n x_i y_i \quad (\text{dot product})$$

The angle between vectors x and y is given by $\cos(\theta) = \frac{\langle x, y \rangle}{\|x\|}$.

With corresponding norm to be the Euclidean Norm

Definition 2.6 – map

Suppose the map $f : \mathbb{R}^n \rightarrow \mathbb{R}$.

Definition 2.7 – differ

We define f to be in C^1, C^2 on an open set $D \subseteq \mathbb{R}^n$, denoted $f \in C^1(D), C^2(D)$, respectively, if the partial first $\frac{\partial f(x)}{\partial x_i}$ and second $\frac{\partial^2 f(x)}{\partial x_i \partial x_j}$ derivatives exist and are continuous for all i, j , respectively. We then get the gradient vector in \mathbb{R}^n and the $n \times n$ symmetric Hessian matrix, respectively denoted as:

$$\nabla f(x) = \left(\frac{\partial f(x)}{\partial x_i} \right) \in \mathbb{R}^n, \quad \nabla^2 f(x) = \left[\frac{\partial^2 f(x)}{\partial x_i \partial x_j} \right] \in \mathbb{S}^n.$$

Here, \mathbb{S}^n is the vector space of $n \times n$ symmetric matrices.

Definition 2.8 – General Nonlinear opt. function NLO

The general problem of nonlinear optimization, denoted NLO, is defined as follows: Given C^2 -smooth functions $f, g_i, h_j : D \subseteq \mathbb{R}^n \rightarrow \mathbb{R}$ for $i = 1, \dots, m$ and $j = 1, \dots, p$, where D is an open subset of \mathbb{R}^n , the objective is to find the optimal value p^* and an optimum x^* of NLO, represented as:

$$p^* := \min f(x) \text{ s.t. } g_i(x) \leq 0, \quad \forall i = 1, \dots, m, h_j(x) = 0, \quad \forall j = 1, \dots, p, x \in D$$

If f, g_i, h_j are all **affine** function and $D = \mathbb{R}^2$, then we have an LP

Definition 2.9 – affine

$$f(x) = Ax + b \quad (1)$$

where $b \neq 0$

Definition 2.10 – Types of Minimality

Consider $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $D \subset \mathbb{R}^n$. Then $\bar{x} \in D$ is:

- a *global minimizer* for f on D if $f(\bar{x}) \leq f(x)$ for all $x \in D$.
- a *strict global minimizer* for f on D if $f(\bar{x}) < f(x)$ for all $x \in D$ where $x \neq \bar{x}$.
- a *local minimizer* for f on D if there exists $\delta > 0$ such that $f(\bar{x}) \leq f(x)$ for all $x \in D \cap B_\delta(\bar{x})$.
- a *strict local minimizer* for f on D if there exists $\delta > 0$ such that $f(\bar{x}) < f(x)$ for all $x \in D \cap B_\delta(\bar{x})$ where $x \neq \bar{x}$.

Definition 2.11 – Linear Approximation

Suppose f is a function that is differentiable on an interval I containing the point a . The **linear approximation** to f at a is the linear function

$$L(x) = f(a) + f'(a)(x - a)$$

for $x \in I$.

Definition 2.12 – Quadratic Approximation

Similar as above, the **quadratic approximation** to f at a is the quadratic function

$$Q(x) = f(a) + f'(a)(x - a) + \frac{1}{2}f''(a)(x - a)^2$$

for $x \in I$.

2.2 Lecture 2**Definition 2.13 – General NLO/NLP**

A **Non-linear Optimization Problem** (NLP) is of the following form:

$$\underbrace{p^*}_{\text{Optimal Value}} = \min \underbrace{f(x)}_{\text{Objective function}}$$

s.t.

$$\begin{aligned} g(x) &= (g_i(x)) \leq 0 \in \mathbb{R}^m \\ h(x) &= (h_j(x)) = 0 \in \mathbb{R}^p \end{aligned}$$

Problem 2.1 – Example

$$\min (x_1 - 2)^2 + (x_2 - 1)^2$$

s.t.

$$\begin{aligned} x_1^2 - x_2 &\leq 0 & (g_1(x) \leq 0) \\ x_1 + x_2 - 2 &\leq 0 & (g_2(x) \leq 0) \end{aligned}$$

Definition 2.14 – Contour

For $\alpha \in \mathbb{R}$, the **contour** of a function f is

$$C_\alpha = \{x \in \mathbb{R}^n : f(x) = \alpha\}$$

Definition 2.15 – Feasible Set

The **feasible set** is

$$F = \{x \in \mathbb{R}^n : g(x) \leq 0, h(x) = 0, x \in D\}$$

(Is D the domain??)

Definition 2.16 – Gradient

The **gradient** of f is

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{pmatrix}$$

For the optimal solution x^* , we have

$$\alpha \nabla f(x^*) = \lambda_1 \nabla g_1(x^*) + \lambda_2 \nabla g_2(x^*)$$

for some $\alpha, \lambda_1, \lambda_2 \in \mathbb{R}$.

We will see later that we can choose $\alpha = 1$ and we need $\lambda_1 \geq 0, \lambda_2 \geq 0$.

Problem 2.2 – Max-cut Problem

Given a weighted graph $G = (\underbrace{V}_{\text{vertices}}, \underbrace{E}_{\text{edges}}, \underbrace{w}_{\text{weight}})$, a **cut** is $U \subseteq V, U \neq \emptyset$. The objective function

$$\max \quad \frac{1}{2} \sum_{\substack{i \in U, j \notin U \\ (i,j) \in E}} w_{i,j}$$

maximizes the sum of edges in a cut.

Formulating as an NLP, we introduce variables $x_i \in \{\pm 1\}, i = 1, \dots, n$. Then the Max-cut problem (MC) is as

follows:

$$\max \quad \frac{1}{2} \sum_{ij \in E} w_{ij}(1 - x_i x_j)$$

Why 1/2 s.t.

$$x_i \in \{\pm 1\} \quad (\text{equivalent to } x_i^2 = 1) \quad \forall i = 1, \dots, n$$

This works because

$$1 - x_i x_j = \begin{cases} 0 & \text{if } x_i = x_j \quad (i, j \text{ in the same set, } U \text{ or } U^c) \\ 2 & \text{otherwise} \end{cases}$$

MC is a **quadratically constrained quadratic program** (QOP) since each constraint $x_i \in \{-1, 1\}$ is equivalent to the quadratic constraint $x_i^2 = 1$. Note that MC is an NP-hard problem.

3 Unconstrained Optimization

3.1 Lecture 2

Problem 3.1 – Simplest Case - No Constraints

Let $\Omega \subseteq \mathbb{R}^n$ be an open set. Assume f is sufficiently smooth (differentiable) then the NLP with no constraints is

$$\min_{x \in \Omega} f(x)$$

Definition 3.1 – Secant Line

A secant line is a line that connects two points on a function.

Theorem 3.1 – Chain Rule (2 dimensions)

Let $f : \mathbb{R}^2 \rightarrow \mathbb{R}$, and two other functions $x(t) : \mathbb{R} \rightarrow \mathbb{R}$ and $y(t) : \mathbb{R} \rightarrow \mathbb{R}$. Let $\phi(t) = f(x(t), y(t))$. The chain rule then states

$$\frac{d\phi}{dt} = \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial y} \frac{dy}{dt}$$

Problem 3.2 – Example of Chain Rule in 2 Dimensions

Let $f(x, y) = x^2 + y^2$. We want to find the rate of change of f along a curve defined by $x(t) = t$ and $y(t) = 2t$. The partial derivatives of f are:

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial f}{\partial y} = 2y$$

The derivatives of $x(t)$ and $y(t)$ are

$$\frac{dx}{dt} = 1, \quad \frac{dy}{dt} = 2$$

Then we get

$$\begin{aligned} \frac{d}{dt} f(x(t), y(t)) &= \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial y} \frac{dy}{dt} \\ &= 2x \cdot 1 + 2y \cdot 2 \\ &= 2(t) \cdot 1 + 2(2t) \cdot 2 \\ &= 10t \end{aligned}$$

Corollary 3.1

Let $f : (a, b) \rightarrow \mathbb{R}$

1. (Necessity) If \bar{x} is a **local minimizer** of f on (a, b) , then $f'(\bar{x}) = 0$ and $f''(\bar{x}) \geq 0$.
2. (sufficient) If $f'(\bar{x}) = 0$, $f''(\bar{x}) > 0$ then \bar{x} is a **strict local minimizer** of f .

Proof.

Since \bar{x} is the local minimizer of f , given small $|\Delta x|$,

$$\begin{aligned} f(\bar{x} + \Delta x) - f(\bar{x}) &\geq 0 \\ f(\bar{x} + \Delta x) &= f(\bar{x}) + f'(\bar{x}) * \Delta x + o(|\Delta x|) \\ f'(\bar{x}) * \Delta x + o(|\Delta x|) &\geq 0 \\ \frac{f'(\bar{x})}{|\Delta x|} * \Delta x + \frac{o(|\Delta x|)}{|\Delta x|} &\geq 0 \end{aligned}$$

Since this holds for all positive and negative Δx . Thus $f'(\bar{x}) = 0$. For the second order proof, we used Taylor thm to construct the contradiction \square

Definition 3.2 – Hessian

The **Hessian** of f at $x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$ is the matrix

$$\nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}$$

Lemma 3.1

Let $v \in \mathbb{R}^n$. Then

$$v = 0 \iff \langle v, d \rangle = 0, \quad \forall d \in \mathbb{R}^n$$

3.2 Lecture 3**Definition 3.3 – Matrix Norm**

$$\|Q\| = \max_{\|x\|=1} \|Qx\| = \text{Largest singular value of } A$$

Theorem 3.2 – Second Order Optimality Conditions (Min)

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be twice continuously differentiable at an open set D . Then

1. Necessary conditions: If \bar{x} is a local minimizer for f on D , then

$$\nabla f(\bar{x}) = 0 \quad \text{and} \quad \nabla^2 f(\bar{x}) \succeq 0$$

2. Sufficient conditions: If $\nabla f(\bar{x}) = 0$, $\nabla^2 f(\bar{x}) \succ 0$ is positive definite then \bar{x} is a strict local minimizer

of f on D .

Proof. This should be proved by the Taylor expansion $f(\bar{x} + \Delta x) = f(\bar{x}) + \nabla f(\bar{x})^T \Delta x + o(\|\Delta x\|)$ □

Theorem 3.3 – Second Order Optimality Conditions (Max)

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be twice continuously differentiable at an open set D . Then

1. Necessary conditions: If \bar{x} is a local maximizer for f on D , then

$$\nabla f(\bar{x}) = 0 \quad \text{and} \quad \nabla^2 f(\bar{x}) \preceq 0$$

2. Sufficient conditions: If $\nabla f(\bar{x}) = 0$, $\nabla^2 f(\bar{x}) \succ 0$ is positive definite then \bar{x} is a strict local maximizer of f on D .

Proof. 1. updated later after I confirmed some details with the professor □

Theorem 3.4

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be twice continuously differentiable and let \bar{x} be a critical point of f . Then

- \bar{x} is a global minimizer if $\nabla^2 f(\mathbf{x}) \succeq 0$ for all $\mathbf{x} \in \mathbb{R}^n$.
- \bar{x} is a strict global minimizer if $\nabla^2 f(\mathbf{x}) \succ 0$ for all $\mathbf{x} \in \mathbb{R}^n$.
- \bar{x} is a global maximizer if $\nabla^2 f(\mathbf{x}) \preceq 0$ for all $\mathbf{x} \in \mathbb{R}^n$.
- \bar{x} is a strict global maximizer if $\nabla^2 f(\mathbf{x}) \prec 0$ for all $\mathbf{x} \in \mathbb{R}^n$.

Definition 3.4 – Critical/Stationary Points

A point $\bar{x} \in U$ is a critical point of a function $f : U \rightarrow \mathbb{R}$ if $\nabla f(\bar{x})$ exists and satisfies $\nabla f(\bar{x}) = 0$.

Problem 3.3 – Algorithm to Find Local Minimizer

Given $f : \mathbb{R} \rightarrow \mathbb{R}$ and $f'(\bar{x}) \neq 0$, then $x_{new} = \bar{x} - (\text{step}) * f'(\bar{x})$.

The idea is that if $f'(\bar{x}) > 0$, then we know that the function is increasing at \bar{x} , so we want to move to the left to obtain the minimum. Similarly, if $f'(\bar{x}) < 0$, then we know that the function is decreasing at \bar{x} , so we want to move to the right to obtain the minimum.

Problem 3.4

Given $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $\phi(\epsilon) = f(\bar{x} + \epsilon d)$

using Taylor expansion $f(\bar{x} + \epsilon d) = f(\bar{x}) + \epsilon \nabla f(\bar{x})^T d + o(\|\epsilon\|)$ shouldnt be ϵd ? or d is the unit vector

let $d = -\nabla f(\bar{x}) / \|\nabla f(\bar{x})\|$, $f(\bar{x}) - \epsilon \|\nabla f(\bar{x})\|^2 + o(\epsilon) < f(\bar{x})$ (if $\nabla f(\bar{x}) \neq 0$)

i.e test nec condition

If $\nabla f(\bar{x}) \neq 0$, then $x_{new} = \bar{x} + \epsilon(-\nabla f(\bar{x}))$ Move to the deepest direction

Definition 3.5 – Cauchy's method of steepest descent

<https://www.math.usm.edu/lambers/mat419/lecture10.pdf> $x_0 \in \mathbb{R}^n$.

$$\|\nabla f(x_k)\| \approx 0? \text{ IF yes Stop}$$

O.W, find a $\alpha > 0$

$$x_{k+1} = x_k - \alpha \nabla f(x_k)$$

repeat

Problem 3.5 – Example of finding global and local minimizers

Find global and local minimizers of $f(x, y) = x^3 - 12xy + 8y^3$.

We first find the gradient and the Hessian:

$$\nabla f(x, y) = \begin{pmatrix} 3x^2 - 12y \\ -12x + 24y^2 \end{pmatrix}$$

$$\nabla^2 f(x, y) = \begin{bmatrix} -6x & -12 \\ -12 & 48y \end{bmatrix}$$

We can find the critical points when we solve for $\nabla f(x, y) = 0$. Solving it, we get solutions $(0, 0)$ or $(2, 1)$.

The Hessian at $(0, 0)$ is

$$\nabla^2 f(0, 0) = \begin{bmatrix} 0 & -12 \\ -12 & 0 \end{bmatrix}$$

The eigenvalues of $\nabla^2 f(0, 0)$ are $-12, 12$. Therefore it is indefinite. So $(0, 0)$ is a saddle point.

The Hessian at $(2, 1)$ is

$$\nabla^2 f(2, 1) = \begin{bmatrix} -12 & -12 \\ -12 & 48 \end{bmatrix}$$

Checking all leading principal minors, we see that they are all positive. So $\nabla^2 f(2, 1)$ is positive definite. So $(2, 1)$ is a local minimizer.

3.3 Lecture 4

Definition 3.6 – Principal Submatrices

Let

$$A = \begin{bmatrix} 1 & 1 & 2 & 7 \\ 1 & 1 & 4 & 6 \\ 2 & 4 & 7 & 8 \\ 7 & 6 & 8 & 1 \end{bmatrix}, \quad I = \{1, 3\}, \quad A[I] = \begin{bmatrix} 1 & 2 \\ 2 & 7 \end{bmatrix}$$

Then $A[I]$ is a **principal submatrix** of A .

Definition 3.7 – Principal Minors

Let $A \in \mathbb{S}^n$, where \mathbb{S}^n is the set of all symmetric $n \times n$ matrices.

1. $\det(A[I])$ is called the **principal minor** of A .
2. If $I = \{1, \dots, k\}$ then $\det(A[I])$ is called the **leading principal minor** of A .

Proposition 3.1 – Characterizing Positive Definiteness with Principal Minors

Let $A \in \mathbb{S}^n$. Then

1. $A \succeq 0 \iff \det(A[I]) \geq 0$ for all principal minors $\det(A[I])$.
2. $A \succ 0 \iff \det(A[I]) > 0$ for all principal minors $\det(A[I])$.
3. $A \succ 0 \iff \det(A[I]) > 0$ for all **leading** principal minors $\det(A[I])$.

Definition 3.8 – Eigenvectors and Eigenvalues

$0 \neq v \in \mathbb{R}^n$ is an **eigenvector** of A if there exists $\lambda \in \mathbb{R}$ such that $Av = \lambda v$. The number λ is called an **eigenvalue** of A .

Theorem 3.5 – Finding Eigenvectors and Eigenvalues

Let A be a matrix.

1. Set up the characteristic equation. We find

$$\det(A - \lambda I) = 0$$

2. Solve for λ . These are the eigenvalues.
3. Plug eigenvalues $\lambda_1, \dots, \lambda_n$ into $(A - \lambda I)v = 0$ and solve for v . These are the eigenvectors.

Theorem 3.6 – Orthogonal Spectral Decomposition

Let $A \in \mathbb{S}^n$. Then A has an **orthogonal spectral decomposition**

$$A = \sum_i \lambda_i u_i u_i^T = U D U^T$$

where U is orthogonal with the orthogonal eigenvectors u_i as columns and D is a diagonal matrix with real eigenvalues on the diagonal.

Corollary 3.2

Let $A \in \mathbb{S}^n$. Then

1. $A \succeq 0$ (positive semidefinite) iff all eigenvalues of A are nonnegative.
2. $A \succ 0$ (positive definite) iff all eigenvalues of A are positive.

Proposition 3.2

Let $A \in \mathbb{S}^n$. The following are equivalent (Positive definite):

1. $A \succ 0$.
2. All the eigenvalues of A are in \mathbb{R}_{++}^n , the interior of the nonnegative orthant.
3. A has a real symmetric positive definite square root, $A = SS$, $S \in \mathbb{S}_{++}^n$.
4. A has a lower triangular factorization, a Cholesky factorization, $A = LL^T$ and L has positive diagonal elements.
5. All principal minors of A are positive.
6. All leading principal minors of A are positive.

And the following are equivalent (Positive semidefinite):

1. $A \succeq 0$.
2. All the eigenvalues of A are in \mathbb{R}_+^n , the nonnegative orthant.
3. A has a real symmetric square root, $A = SS$, $S \in \mathbb{S}^n$.

4. A has a lower triangular factorization, a Cholesky factorization, $A = LL^T$.
5. All principal minors of A are nonnegative.

Problem 3.6 – Motivation

When can we guarantee that global minimizers of $f : \mathbb{R}^n \rightarrow \mathbb{R}$ exist?

For example, the real valued function on \mathbb{R} $f(x) = e^x$ is bounded below by 0 but has no minimizers. The minimum value is 0 but is not attained.

Proposition 3.3 – Weierstrass Extreme Value Theorem

If $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is continuous, and if $D \subset \mathbb{R}^n$ is a compact set (closed and bounded), then f attains its global maximum and minimum on D .

Problem 3.7 – Example of a continuous function that does not attain its minimum

Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be defined by $f(x) = e^x$. Then f is continuous, but $D = \mathbb{R}$ is not compact (closed but not bounded). We can see that f does not have any global minimizer.

Definition 3.9 – Coercive function

A continuous function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is **coercive** if for any sequence x_i with $\|x_i\| \rightarrow \infty$, it must be the case that $f(x_i) \rightarrow +\infty$. In other words,

$$\lim_{\|x\| \rightarrow \infty} f(x) = +\infty$$

Here are some examples:

1. $f_1(x) = x^2$ is coercive.
2. $g(x) = x$ is not coercive (because as $x \rightarrow -\infty$, $g(x) \rightarrow -\infty \neq \infty$).
3. $h(x) = e^x$ is not coercive.

Proposition 3.4 – Coercive Functions and Minimizers

A coercive function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ has a global minimizer.

Definition 3.10 – Level Sets

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a function and let $\alpha \in \mathbb{R}$. An α -level set of f is defined by

$$L_\alpha = \{x \in \mathbb{R}^n : f(x) = \alpha\}$$

That is, all points x such that $f(x) = \alpha$.

- When $n = 2$, we call this a level curve.
- When $n = 3$, we call this a level surface.
- When $n > 3$, we call this a level hypersurface.

Definition 3.11 – Sub-level set

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a function and let $\alpha \in \mathbb{R}$. An α -sublevel set of f is defined by

$$S_\alpha(f) = \{x \in \mathbb{R}^n : f(x) \leq \alpha\}$$

That is, all points x below the line $f(x) = \alpha$.

Problem 3.8

Can we find minimizer for $q : \mathbb{R}^n \rightarrow \mathbb{R}$. $q(x) = \frac{1}{2}x^T Qx + b^T x + \alpha$ ($Q = Q^T$)

Let $p^* = \inf q(x)$

- When is it finite?
- When is it attained?

Proposition 3.5 – bdd blow Need to confirm

$q(x)$ is bdd below iff $Q \succeq 0$ and $b \in \text{Range}(Q)$ and $0 = \nabla q(x) = Qx - b$ so $x^* = Q^{-1}b$ is Orthogonal (why) so always attained

Proof. Since Q is positive semidef, we can use spectral decomposition, $Q = UDU^T$, $U^T U = I$. $x^T Qx = x^T UDU^T x$ which is also a quadratic form, let $y = U^T x$, $x = Uy$

Thus for $q(x)$, we sub $x = Uy$, then we get

$$\begin{aligned} q(x) &= \frac{1}{2}(Uy)^T Q(Uy) + b^T Uy + \alpha \\ &= \frac{1}{2}y^T D y + (U^T b)^T y + \alpha \text{ Let } \bar{b} = U^T b \\ &= \sum \lambda_i y_i^2 + \bar{b}_i y_i + \alpha \end{aligned}$$

Which is a separable problem. $p_i^* = \min \frac{1}{2}\lambda_i y_i^2 + \bar{b}_i y_i$
 p_i^* is finite iff $\lambda_i \geq 0$, $\lambda_i = 0 \implies \bar{b}_i = 0$ Why. $\bar{b}_i = u_i^T b$ which is the i th eigenvector. □

Theorem 3.7 – Weierstrass

Given $f: \mathbb{R}^n \rightarrow \mathbb{R}$ cts and D in \mathbb{R}^n closed and bounded, Then $\exists \bar{x} \in D$ s.t $\bar{x} \in \text{argmin } f(x)$

Proposition 3.6

If f is coercive, f maps \mathbb{R}^n to \mathbb{R} and cts, then there exists $\bar{x} \in \text{argmin } f(x)$

Proof. Omit □

Theorem 3.8 – $q(x)$ is coercive iff Q is positive definite

Proof. Omit □

4 Linear Least Squares & Solving Linear Systems

4.1 Lecture 5

Problem 4.1 – Motivation For Least Squares

Suppose we have a series of observed values from an experiment:

$$\{(t_1, s_1), (t_2, s_2), \dots, (t_m, s_m)\}$$

where t_i is the time and s_i is the observed value at time t_i . We want to find a polynomial function

$$p(t) = x_0 + x_1 t + \dots + x_n t^n$$

that fits the data. So we want to find coefficients x_0, \dots, x_n such that $p(t_i) \approx s_i$ for all i . More formally, we want to minimize the absolute value of the error of each term. The error (ℓ_1 norm) is defined as

$$|e_i| = |p(t_i) - s_i|$$

This can be formulated into a ℓ_1 norm minimization problem:

$$\min \left\{ \sum_{i=1}^m |p(t_i) - s_i| : (x_0, \dots, x_n) \in \mathbb{R}^{n+1} \right\}$$

This is a non-differentiable optimization problem since we have absolute values which make it not smooth. So we can reformulate it as a linear program:

$$\min \sum_{i=1}^m \lambda_i$$

s.t.

$$\begin{aligned} s_i - p(t_i) &\leq \lambda_i && \text{for all } i = 1, \dots, m \\ p(t_i) - s_i &\leq \lambda_i && \text{for all } i = 1, \dots, m \end{aligned}$$

This minimization problem is called **compressive sensing**.

Definition 4.1 – Vandermonde Matrix

Let

$$A = \begin{bmatrix} 1 & t_1 & t_1^2 & \dots & t_1^n \\ 1 & t_2 & t_2^2 & \dots & t_2^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & t_m & t_m^2 & \dots & t_m^n \end{bmatrix} \in \mathbb{R}^{m \times (n+1)}, \quad b = \begin{pmatrix} s_1 \\ s_2 \\ \vdots \\ s_m \end{pmatrix}, \quad x = \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{pmatrix}$$

A is called a **Vandermonde matrix**.

Theorem 4.1

The Vandermonde Matrix

$$A = \begin{bmatrix} 1 & t_1 & t_1^2 & \cdots & t_1^n \\ 1 & t_2 & t_2^2 & \cdots & t_2^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & t_m & t_m^2 & \cdots & t_m^n \end{bmatrix} \in \mathbb{R}^{m \times (n+1)}, \quad b = \begin{pmatrix} s_1 \\ s_2 \\ \vdots \\ s_m \end{pmatrix}, \quad x = \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{pmatrix}$$

is full column rank if $n + 1 \leq m$ and the points t_i are distinct.

Definition 4.2 – ℓ_1 and ℓ_2 Norm

The ℓ_1 norm of a vector x is defined to be

$$\|x\| = \sum |x_i|$$

The ℓ_2 norm of a vector x is defined to be

$$\|x\| = \sqrt{\sum x_i^2}$$

Problem 4.2 – Linear Least Squares Problem

Recall our ℓ_1 norm minimization problem:

$$\min \left\{ \sum_{i=1}^m |p(t_i) - s_i| : (x_0, \dots, x_n) \in \mathbb{R}^{n+1} \right\}$$

We can instead use ℓ_2 norm defined as $\|e\|_2 = \sqrt{\sum e_i^2}$. So our ℓ_2 minimization problem is

$$\min \left\{ \sum_{i=1}^m (p(t_i) - s_i)^2 : (x_0, \dots, x_n) \in \mathbb{R}^{n+1} \right\}$$

where $p(t) = x_0 + x_1 t + \cdots + x_n t^n$. Using the Vandermonde matrix, we can rewrite our problem to be

$$\min \frac{1}{2} \|Ax - b\|^2$$

where

$$A = \begin{bmatrix} 1 & t_1 & t_1^2 & \cdots & t_1^n \\ 1 & t_2 & t_2^2 & \cdots & t_2^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & t_m & t_m^2 & \cdots & t_m^n \end{bmatrix} \in \mathbb{R}^{m \times (n+1)}, \quad b = \begin{pmatrix} s_1 \\ s_2 \\ \vdots \\ s_m \end{pmatrix}, \quad x = \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{pmatrix}$$

The objective function is $g(x) = \frac{1}{2} \|Ax - b\|^2$. Let's first expand $g(x)$:

$$\begin{aligned} g(x) &= \frac{1}{2} \|Ax - b\|^2 \\ &= \frac{1}{2} (Ax - b)^T (Ax - b) \\ &= \frac{1}{2} (Ax)^T Ax - (Ax)^T b + \frac{1}{2} \|b\|^2 \\ &= \frac{1}{2} x^T A^T Ax - x^T A^T b + \frac{1}{2} \|b\|^2 \end{aligned}$$

Then, using the definition of linear transformation definition of the gradient (WTF is this (This is the matrix differentiation. I think there are only three forms and just remember them lolll<https://atmos.washington.edu/dennis/MatrixCalculus.pdf>)), we have

$$\nabla g(x) = A^T Ax - A^T b$$

To find the critical points, we solve for $\nabla g(x) = 0$. So the critical points are x^* that satisfy the equation

$$A^T Ax = A^T b$$

This is also called a **normal equation**.

also something about the condition number, i dont really understand.

Definition 4.3 – Singular Values of a Matrix

The singular values of a matrix A are the square roots of the eigenvalues of the matrix $A^T A$. They are always non-negative real numbers.

The number of non-zero singular values of a matrix equals the rank of that matrix.

Definition 4.4 – Condition Number of a Matrix

Suppose $A \in \mathbb{R}^{m \times n}$, $m > n$ is full column rank. The condition number of the matrix A , $\text{cond}(A)$, is the ratio of the largest to smallest nonzero singular values of A . Let σ_{\max} be the largest singular value and σ_{\min} be the smallest singular value. Then

$$\text{cond}(A) = \frac{\sigma_{\max}}{\sigma_{\min}}$$

Definition 4.5 – Frechet Derivative

Let $h : U \rightarrow W$, where U is an open subset of V , and V, W are finite dimensional vector spaces. The function h is **Frechet differentiable** at $x \in U$ if there exists a linear transformation $A : V \rightarrow W$ such that

$$\lim_{d \rightarrow 0} \frac{\|h(x+d) - h(x) - Ad\|}{\|d\|} = 0$$

idk

4.2 Lecture 6

Goal: Solving normal equation/non linear case

Definition 4.6 – SVD Decomposition

Let A be an $m \times n$ matrix. Then A can be factored into

$$\underbrace{A}_{m \times n} = \underbrace{U}_{m \times m} \underbrace{\Sigma}_{m \times n} \underbrace{V^T}_{n \times n}$$

where

- U is an $m \times m$ orthogonal matrix consisting of eigenvectors of AA^T
- V^T is the transpose of an $n \times n$ matrix containing the eigenvectors of $A^T A$
- Σ is a diagonal matrix with $r = \text{rank}(A)$ positive eigenvalues of AA^T (Singular values of A) on the diagonal.

there is a section on piazza posted lecture notes that shows why using SVD decomposition to solve normal equation is a bad idea. Not sure if i should include here

Definition 4.7 – Orthogonal Matrix

A matrix Q is orthogonal if $Q^T Q = I$.

Definition 4.8 – Orthonormal Columns

A matrix Q has orthonormal columns if each column vector is a unit vector (norm is 1), and any two distinct columns are orthogonal (inner product is 0).

Problem 4.3**Applicable Model for "best" data fitting**

$$(s_i, p_i), \quad i = 1, \dots, m$$

We got linear model and we need to solve $A^T A x = A^T b$ normal equation

Today: Solve normal equation (whenever case)

i.e., this is from optimality condition for

$$\min \frac{1}{2} \|Ax - b\|_2^2 = f(x)$$

$$, \text{ s.t. } A \in M_{m,n}$$

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

$$\text{stationary: } \nabla f(\bar{x}) = A^T (A\bar{x} - b) = 0$$

An alternate view is $\min \|y - b\|$

, s.t. $y \in \text{Range}(A) \Rightarrow$ a projection problem

i.e., project b onto $\text{Range of } A$

$$\text{Aside: use SVD of } A = U\Sigma V^T : \Sigma = \begin{bmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_r \\ & 0 & \end{bmatrix}, \quad r = \text{rank}(A) \quad \sigma_i > 0$$

SVD can be used for a "rank revealing" decomposition.

$$U = [U_1 \quad U_2]$$

Where:

$U_1 : m \times r$ orthogonal columns span $\mathcal{R}(A)$

$U_2 : m \times (m-r)$ spanning $\mathcal{N}(A^T)$

Properties:

$$U^T U = I \quad \text{and} \quad I = U_1^T U_1 = (U_1^T U_1)^T = \mathcal{C}(U_1 U_1^T) = U_1 U_1^T$$

This means $U_1 U_1^T$ is symmetric idempotent, i.e., orthogonal projection.

To solve the projection minimizing $\|y - b\|$ where $y \in \text{Range}(\mathcal{R}(A))$:

$$\text{optimal } y^* = U_1 U_1^T b$$

Defining the Moore-Penrose generalized inverse:

$$A^+ = V \Sigma^+ U^T$$

where

$$\Sigma^+ = \begin{bmatrix} \frac{1}{\sigma_1} & \cdots & 0 \\ 0 & \cdots & 0 \end{bmatrix}$$

and

$$\gamma_i = \frac{b_i}{\sigma_i} \quad \text{if } \sigma_i \neq 0$$

Finally, to find x such that $Ax = y^* = U_1 U_1^T b = AA^+ b$: If A has full column rank (i.e., $\mathcal{R}(A^T) = \mathbb{R}^n$), then x is unique. Otherwise $\bar{x} + v, v \in N(A)$ is a solution for all v in $N(A)$. Choosing a large solution. This solution of min is called "Best least square solution"

we can write it as bilevel problem

The solution of minimum norm is called the "best least square solution". This can be represented as a "bilevel problem":

$$\min_{\hat{x}} \|\hat{x}\|_2 \quad \text{for values when different}$$

subject to:

$$x \in \arg \min_z \frac{1}{2} \|Ax - b\|_2^2$$

The bLSS (best least square solution) is the unique LSS (least square solution) in $\mathcal{R}(A^T)$.

Definition 4.9 – Condition number

Given:

$$A = U\Sigma V^T \quad (\text{SVD of } A)$$

Where Σ is a diagonal matrix with:

$$\Sigma = \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_r \end{pmatrix} \quad \text{and} \quad \sigma_r \geq 0$$

The condition number of matrix A is given by:

$$\text{Cond}(A) = \frac{\sigma_1}{\sigma_r}$$

If A is not of full rank, then:

$$\text{Cond}(A) = \infty \implies \text{Cond}(A^T) = \text{Cond}(A)$$

We also have:

$$A^T A = V\Sigma^T U^T U\Sigma V^T = V\Sigma^2 V^T$$

With:

$$\Sigma^2 = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_r^2 \end{pmatrix}$$

Thus:

$$\text{Cond}(A^T A) = \frac{\sigma_1^2}{\sigma_r^2} = \text{Cond}(A)^2$$

For the solution B :

$$Bx^*(\text{True sol}) = b, B\hat{x}(\text{Numerical}) = b + \delta b$$

Where:

$$\frac{\|x^* - \hat{x}\|}{\|x^*\|} \leq \text{Cond}(B) \frac{\delta \|b\|}{\|b\|}$$

To avoid solving the normal equation with squares condition number, we should use QR

Definition 4.10 – QR Factorization

For any $m \times n$ matrix A , there exists an $m \times m$ orthogonal matrix Q ($QQ^T = I$) and an $m \times n$ upper triangular matrix R ($R_{i,j} = 0, \forall i < j$) satisfying $A = QR$. Moreover, if the columns of A are linearly independent then we can get

$$\begin{aligned} A &= QR \\ &= Q \begin{bmatrix} R_1 \\ 0 \end{bmatrix} \\ &= [Q_1 \quad Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} \\ &= Q_1 R_1 \end{aligned}$$

where

- R_1 is an invertible $n \times n$ upper triangular matrix
- 0 is an $(m - n) \times n$ zero matrix
- Q_1 is an $m \times n$ matrix with orthonormal columns
- Q_2 is an $m \times (m - n)$ matrix with orthonormal columns

Theorem 4.2 – QR Factorization on Normal Equation

Assuming that the columns of A are linearly independent, then the normal equation $A^T A x = A^T b$ can be solved by applying QR factorization to A :

$$\begin{aligned} (A^T A)x &= A^T b \\ ((Q_1 R_1)^T Q_1 R_1)x &= (Q_1 R_1)^T b \\ (R_1^T Q_1^T Q_1 R_1)x &= R_1^T Q_1^T b \\ R_1^T R_1 x &= R_1^T Q_1^T b && \text{Since } Q_1 \text{ is orthogonal} \\ R_1 x &= Q_1^T b && \text{Since } R_1 \text{ is invertible} \end{aligned}$$

Definition 4.11 – Methods of Solving General Linear Systems

Suppose we are given a linear system $Bx = b$, and we know that this system has a solution, i.e. $b \in \text{range}(B)$. There are 3 important algorithms/factorizations used to find x :

- Gaussian Elimination (LU factorization) ($PB = LU$)
- QR factorization
- SVD, singular value decomposition

Problem 4.4 – Solving Large Positive Definite Systems

Suppose we have a linear system, $Ax = b$, with A positive definite. If x^* is a solution, then $Ax^* - b = 0$. Then this is equivalent to minimizing the function

$$f(x) = \frac{1}{2} \|Ax - b\|^2, \nabla f(x) = Ax - b = 0$$

Dont understand this and the part after as well. You will have to add more notes here. Link to notes [HERE](#)

Definition 4.12 – Steepest Descent Direction in First order model

The steepest descent direction in the first order model is $d = -\frac{\nabla f(x_c)}{\|\nabla f(x_c)\|}$

Theorem 4.3 – Conjugate Gradient Method

The first search direction is the negative gradient,

$$v_0 = -\nabla q(x_0)$$

with $q = f$. At the k th iteration:

$$v_{k+1} = -\nabla q(x_k) + \beta_k v_k$$

where β_k is chosen to ensure $\langle Av_{k+1}, v_k \rangle = 0$. This guarantees that the directions are A -conjugate **wtf is A conjugate u, v conjugate, if $u^T A v = 0$** . We then set

$$x_{k+1} = x_k + \alpha_{k+1} v_{k+1}$$

where α_{k+1} is chosen from an exact line search (**what is line search**).

Problem 4.5

$$\min_{x \in D \subset \mathbb{R}} f(x)$$

- 1st & 2nd order optimality condition both necessary and sufficient
- 1st, 2nd order model

4.3 Lecture 7**Definition 4.13 – Nonlinear Least Square**

Suppose we have $F : \mathbb{R}^n \rightarrow \mathbb{R}^m$ where

$$F(x) = \begin{pmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_m(x) \end{pmatrix}$$

Then the nonlinear least squares problem is

$$\min \{h(x)\}$$

where

$$h(x) = \frac{1}{2} \|F(x)\|^2 = \frac{1}{2} \langle F(x), F(x) \rangle = \frac{1}{2} \sum_{i=1}^m f_i^2(x)$$

Definition 4.14 – Jacobian Matrix

Let F be defined as above, then the Jacobian matrix is $J(x) = F'(x)$ where

$$F'(x) = \begin{bmatrix} \nabla f_1(x)^T \\ \nabla f_2(x)^T \\ \vdots \\ \nabla f_m(x)^T \end{bmatrix}$$

Problem 4.6 – Solving Nonlinear Least Squares

For the nonlinear least squares problem defined above, we consider the special case $m = n$. Then we can consider the problem as solving the square system of nonlinear equations $F(x) = 0$. Recall that for current approximation x_c ,

$$0 = F(x_c + d) \approx F(x_c) + \underbrace{F'(x_c)}_{\text{Jacobian}} \underbrace{d}_{\text{search direction}}$$

So we solve

$$F'(x_c)d = -F(x_c)$$

which is called the Newton equation. Then we can take a step in the search/Newton direction d to get a new approximation $x_{c+1} = x_c + \alpha d$ for appropriate step length α .

In general, $\nabla h(x_c) = \sum_{i=1}^m f_i(x_c) \nabla f_i(x_c) = J(x_c)^T F(x_c)$

Definition 4.15 – Second Order Model for Nonlinear Problem

$h(x + \nabla x) \sim h(x) + \frac{1}{2} \nabla^2 h(x) \nabla x$ **upload later**

Definition 4.16 – Argmin and argmax

argmin $f(x)$ is the set of all minimizers of $f(x)$, similarly argmax $f(x)$ is the set of all maximizers of $f(x)$.

Theorem 4.4 – Lagrange Multipliers for Equality Constraints

Suppose that $f : C \rightarrow \mathbb{R}$ and $h : C \rightarrow \mathbb{R}^m$ are sufficiently smooth functions on the open set $C \subseteq \mathbb{R}^n$. Let $x \in C$ be a local minimum of f subject to the constraints $h(x) = 0, x \in C$. In addition, assume the following regularity condition at x (constraint qualification at x)

$$h'(x) \text{ is onto}$$

Then there exists $\lambda \in \mathbb{R}^m$ (a Lagrange multiplier vector) such that

$$0 = \nabla f(x) + \langle \lambda, h'(x) \rangle$$

Equivalently, the gradient $\nabla f(x)$ is in the range of $h'(x)^T$.

Problem 4.7 – DNE of multiplier

Recall:

minimize $f(x)$
subject to $f_i(x) = 0, \quad i = 1, \dots, m$

$$L(x, \lambda) = f(x) - \sum_{i=1}^m \lambda_i f_i(x) \quad (\text{Lagrangian multiplier})$$

If x^* is a local minimum and

$\{\nabla f_i(x^*)\}$ is a linearly independent set, then $\nabla L(x^*, \lambda) = \nabla f(x^*) + \sum_{i=1}^m \lambda_i \nabla h_i(x^*) = 0$ for some $\lambda \in \mathbb{R}$

Example:

$$\begin{aligned} f(x) &= x \\ h(x) &= x^2 = 0 \\ L(x, \lambda) &= x + \lambda x^2, \quad \text{with constraint } x^2 = 0 \\ 0 &= \nabla L(x, \lambda) = 1 + 2\lambda x = 1 + 0. \text{ No } \lambda \text{ exist} \end{aligned}$$

5 Iterative Methods for Unconstrained Optimization

5.1 Lecture 8-10

Before, we have iterative methods to solve linear and linear least squares system.

Goal: Solve more general problems of minimization.

An iterative algorithm is a procedure that produces an (infinite) sequence of points $\{x_k\}$, in \mathbb{R}^n such that our sequence converges to a critical point of f or to a point that satisfies the second order necessary conditions of optimality.

5.1.1 Line Search Strategy

Most Line Search Algorithms have the following procedure:

Choose a starting point x_0 . For $k = 0, 1, 2, \dots$

1. Choose a search direction d_k .
2. Choose a step length $\alpha_k > 0$ (that satisfies $f(x_k + \alpha_k d_k) < f(x_k)$)
3. Update $x_{k+1} = x_k + \alpha_k d_k$
4. Stop if a stopping criterion is satisfied.

Definition 5.1 – Line Search Strategy

At each iteration k , we choose a vector (search direction) $d_k \neq 0 \in \mathbb{R}^n$, then choose $\alpha_k > 0$ (step length) that approximately solves

$$\alpha_k \in \operatorname{argmin} f(x_k + \alpha d_k)$$

Then we update $x_{k+1} = x_k + \alpha_k d_k$.

5.1.1.1 Finding Descent Direction

Definition 5.2 – Descent Direction

Let $x \in U \subseteq \mathbb{R}^n$ with U being an open set. Then $d \in \mathbb{R}^n$ is a descent direction for f at x if there exists $\bar{\alpha} > 0$ such that

$$x + \alpha d \in U, f(x + \alpha d) < f(x)$$

for all $0 < \alpha < \bar{\alpha}$.

So $f(x_{k+1}) < f(x_k)$.

Lemma 5.1

Let f be sufficiently smooth on an open set U and let $\bar{x} \in U$. Let $d \in \mathbb{R}^n$ satisfy

$$\langle d, \nabla f(\bar{x}) \rangle = \nabla f(\bar{x})^T d < 0$$

Then d is a descent direction for f at \bar{x} .

(i.e., the directional derivative of f at \bar{x} in the direction of d is negative, so we know that it is the descent direction.)

Proof. **Proof.** From the hypothesis we have

$$f(x + td) = f(x) + t\nabla f(x) \cdot d + o(t).$$

Therefore we deduce

$$\frac{f(x + td) - f(x)}{t} = \langle d, \nabla f(x) \rangle + \frac{o(t)}{t} < 0, \text{ for all sufficiently small } t > 0.$$

Moreover, since U is open, we have $x + td \in U$ for all sufficiently small $t > 0$. □

□

Problem 5.1 – Example(direction of steepest descent)

We saw

$$\min \nabla f(x)^T \cdot d \quad \text{s.t.} \quad \|d\| = 1$$

get

$$d = -\frac{\nabla f(x)^T}{\|\nabla f(x)\|}$$

Cauchy direction of steepest descent

Alternatively,

$$-\nabla f(x)^T \cdot d \leq \|d\| \cdot \|\nabla f(x)^T\| = \|d\| \cdot \|\nabla f(x)\|$$

but

$$d = -\nabla f(x)^T \text{ gives equality.}$$

So C.S yields s.t direction

If $B \succ 0$, then

$$d = -B^{-1}\nabla f(x)^T \text{ in a "deflated gradient" direction.}$$

Proposition 5.1 – Existence of B

Suppose $\nabla f(\bar{x})^T d < 0$. Then there exists $B \succ 0$ that satisfies $d = -B^{-1}\nabla f(\bar{x})$

Proof. Ignore it for now text □

5.1.2 Second order model: Newton Type

Model $m_q(x) = f(x_c) + \nabla f(x_c)^T \Delta x + \frac{1}{2} \Delta x^T B_c \Delta x$ where $B_c \simeq \nabla^2 f(x_c)$

Lemma 5.2 – TFAE

1. $m_q(\Delta x)$ is bdd below
2. $B_c \succeq 0$ and $\nabla f(x_c) \in \text{range}(B_c)$
3. $\Delta \bar{x} = -B_c^+ \nabla f(x_c)$ is a global minimum of m_q

Proof. 2 to 1:

Suppose 2 holds, we have $B_c \succeq 0$ and $\exists \bar{\Delta}x, B_c \bar{\Delta}x = -\nabla f(x_c)$. This is also the stationary condition. Again, since B_c is psd, there exists a psd square root such that $ss = B_c$.

Then lets complete the square

$$mq(\Delta x) =$$

confirm

□

The main difference between line search methods is the choice of the descent direction

Problem 5.2 – Example

If $\nabla f(x) \neq 0$ then $d = -\nabla f(x)$ is a descent direction since

$$d^T \nabla f(x) = -\nabla f(x)^T \nabla f(x) = -\|\nabla f(x)\|_2^2 < 0$$

Another option is letting $d = -H^{-1} \nabla f(x)$ where $H \succ 0$ and $\nabla f(x) \neq 0$ since

$$d^T \nabla f(x) = -\nabla f(x)^T H^{-1} \nabla f(x) < 0$$

since $H \succ 0$, we have $H^{-1} \succ 0$, so $\nabla f(x)^T H^{-1} \nabla f(x) > 0$.

Theorem 5.1 – Existence of a Descent Direction

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be continuously differentiable and let $\bar{x} \in \mathbb{R}^n$. Assume that d is a descent direction of f at \bar{x} , so

$$\nabla f(\bar{x})^T d < 0$$

Then there exists $\delta > 0$ such that for every $\alpha \in (0, \delta]$,

$$f(\bar{x} + \alpha d) < f(\bar{x})$$

Proof. By Taylor's theorem, for all $x \in \mathbb{R}^n$,

$$f(x) = f(\bar{x}) + \nabla f(\bar{x})^T (x - \bar{x}) + o(\|x - \bar{x}\|)$$

Then

$$f(\bar{x} + \alpha d) = f(\bar{x}) + \nabla f(\bar{x})^T (\bar{x} + \alpha d - \bar{x}) + o(\|\bar{x} + \alpha d - \bar{x}\|)$$

Simplifying gives

$$f(\bar{x} + \alpha d) = f(\bar{x}) + \underbrace{\alpha \nabla f(\bar{x})^T d}_{< 0} + o(\|\alpha d\|)$$

Rearranging and dividing both sides by $\alpha \|d\|$, we get

$$\frac{f(\bar{x} + \alpha d) - f(\bar{x})}{\alpha \|d\|} = \frac{\nabla f(\bar{x})^T d}{\|d\|} + \frac{o(\|\alpha d\|)}{\alpha \|d\|}$$

Taking the limit as $\alpha \rightarrow 0$, we get

$$\lim_{\alpha \rightarrow 0} \frac{f(\bar{x} + \alpha d) - f(\bar{x})}{\alpha \|d\|} = \frac{\nabla f(\bar{x})^T d}{\|d\|}$$

Since $\nabla f(\bar{x})^T d < 0$, we know that the limit is negative. Then there exists $\delta > 0$ such that for all $\alpha \in (0, \delta]$, we have

$$\frac{f(\bar{x} + \alpha d) - f(\bar{x})}{\alpha \|d\|} < 0$$

□

5.1.2.1 Finding Step Size

The process of finding the step size α_k is called line search. Some common choices for step size are as follows:

1. $\alpha_k = \alpha$ (a constant) for every k
2. Exact line search: $\alpha_k = \operatorname{argmin}_{\alpha \geq 0} f(x_k + \alpha d_k)$
3. Inexact line search: A step size α_k that achieves a sufficient decrease in f . One popular inexact line search conditions are called the Wolfe conditions.

Problem 5.3 – Exact Line Search

For exact line search, we define a new function

$$\phi(\alpha) = f(x_k + \alpha d_k)$$

We can differentiate w.r.t. α using the chain rule to obtain

$$\phi'(\alpha) = \nabla f(x_k + \alpha d_k)^T d_k$$

Then we set $\phi'(\alpha) = 0$ to obtain the critical point of ϕ . Then we can use the second derivative test to determine if the critical point is a local minimizer. If it is, then we have found the optimal step size α_k .

Definition 5.3 – Wolfe Conditions

Let $0 < c_1 < c_2 < 1$. The Wolfe conditions are

1. Sufficient decrease condition:

$$f(x_k + \alpha d_k) \leq f(x_k) + c_1 \alpha \nabla f(x_k)^T d_k$$

or equivalently

$$\phi(\alpha_k) \leq \phi(0) + c_1 \alpha \phi'(0)$$

2. Curvature condition:

$$\nabla f(x_k + \alpha d_k)^T d_k \geq c_2 \nabla f(x_k)^T d_k$$

or equivalently

$$\phi'(\alpha_k) \geq c_2 \phi'(0)$$

Theorem 5.2 – Existence of Step Lengths that Satisfy Wolfe Conditions

Assume $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is continuously differentiable. Let d_k be a descent direction at x_k and assume f is bounded below along the ray $\{x_k + \alpha d_k : \alpha \geq 0\}$. Then if $0 < c_1 < c_2 < 1$ there exist intervals of step lengths satisfying the Wolfe conditions.

Proof. Omitted □

5.1.2.2 Steepest Descent Method

The steepest descent method is easy to implement as it requires the calculation of the gradient but not second derivatives. The descent direction at each iteration is chosen as

$$d_k = -\nabla f(x_k)$$

Lemma 5.3

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be continuously differentiable and let $\bar{x} \in \mathbb{R}^n$ such that $\nabla f(\bar{x}) \neq 0$. Then the optimal solution of the following minimization problem

$$\min_{d \in \mathbb{R}^n} \{ \nabla f(\bar{x})^T d : \|d\|_2 = 1 \}$$

is

$$d^* = \frac{-\nabla f(\bar{x})}{\|\nabla f(\bar{x})\|_2}$$

Proof. By Cauchy-Schwarz inequality, we have

$$\nabla f(\bar{x})^T d \geq -\|\nabla f(\bar{x})\|_2 \|d\|_2 = -\|\nabla f(\bar{x})\|_2$$

The smallest value of d is $d = \frac{-\nabla f(\bar{x})}{\|\nabla f(\bar{x})\|_2}$ since if we plug in d into the inequality, we get

$$\nabla f(\bar{x})^T \frac{-\nabla f(\bar{x})}{\|\nabla f(\bar{x})\|_2} = \frac{-\|\nabla f(\bar{x})\|_2^2}{\|\nabla f(\bar{x})\|_2} = -\|\nabla f(\bar{x})\|_2$$

So $d^* = \frac{-\nabla f(\bar{x})}{\|\nabla f(\bar{x})\|_2}$ is a minimizer of this problem. □

Theorem 5.3

Let $\{x_k\}$ be the sequence generated by the method of steepest descent method where the step sizes are chosen by the exact line search. Then for every $k \geq 0, k \in \mathbb{N}$

$$(x_{k+2} - x_{k+1})^T (x_{k+1} - x_k) = 0$$

5.1.2.3 Backtracking Line Search**Definition 5.4 – Backtrack Inexact Line Search**

We make use of the Wolfe Conditions.

1. Initialize $\alpha > 0$, for example, choose $\alpha = 1, c \in (0, 1)$
2. if $(\phi(\alpha) > \phi(0) + c\alpha\phi'(0))$
 - (a) while $(\phi(\alpha) > \phi(0) + c\alpha\phi'(0))$
 - i. $\alpha = \alpha/2$
3. else if $(\phi(2\alpha) \leq \phi(0) + 2c\alpha\phi'(0))$
 - (a) while $(\phi(2\alpha) \leq \phi(0) + 2c\alpha\phi'(0))$
 - i. $\alpha = 2\alpha$
4. Output = α .

5.1.2.4 Newton's Method

In Newton's Method, the search direction is given by

$$d_k = -[\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$$

The Newton step is defined only when $\nabla^2 f(x_k)$ is positive definite.

Definition 5.5 – Newton’s Method

Input: Initial point: x_0 , Tolerance: $\epsilon > 0$

1. Solve the linear system of equations $\nabla^2 f(x_k) d_k = -\nabla f(x_k)$ for d_k , so $d_k = -[\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$
2. Update $x_{k+1} = x_k + \alpha_k d_k$ where $\alpha_k = 1$ for Newton’s method
3. If $\|\nabla f(x_{k+1})\|_2 \leq \epsilon$, stop. Otherwise, go to step 1.

Definition 5.6 – Operator Norm

The operator norm of a matrix $Q \in \mathbb{R}^{m \times n}$ is defined by

$$\|Q\|_2 = \max\{\|Qx\|_2 : x \in \mathbb{R}^n, \|x\|_2 = 1\}$$

This definition satisfies the properties of the norm. For every $A \in \mathbb{R}^{m \times n}$,

- $\|A\|_2 = 0 \iff A = 0$
- $\|\alpha A\|_2 = |\alpha| \|A\|_2$ for every $\alpha \in \mathbb{R}$
- $\|A + B\|_2 \leq \|A\|_2 + \|B\|_2$

Theorem 5.4

For every $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^n$, we have

$$\|Ax\|_2 \leq \|A\|_2 \|x\|_2$$

5.1.2.5 Quasi-Newton Methods

Since computing the Hessian matrix is expensive, we can use an approximation of the Hessian matrix instead. We now set the search direction as

$$d_k = -B_k^{-1} \nabla f(x_k)$$

where the symmetric and positive definite matrix B_k is updated at every iteration by a quasi-Newton updating formula.

There are many quasi-Newton methods, but we will only discuss the BFGS method.

Consider the quadratic model of the objective function:

$$m_k(d) = f(x_k) + \nabla f(x_k)^T d + \frac{1}{2} d^T B_k d$$

where B_k is a positive definite matrix and will be updated at every iteration. The minimizer of this quadratic model is

$$d_k = -B_k^{-1} \nabla f(x_k)$$

It is used as the search direction and the new iterate is given by

$$x_{k+1} = x_k + \alpha_k d_k$$

where α_k is the step length, chosen so that it satisfies the Wolfe conditions. In this method, we match the gradient of m_{k+1} to the gradient of f at x_k and x_{k+1} . That is, we require

$$\nabla m_{k+1}(0) = \nabla f(x_{k+1})$$

$$\nabla m_{k+1}(-\alpha_k d_k) = \nabla f(x_k)$$

From the second equation above, we get

$$\nabla_{k+1}(-\alpha_k d_k) = \nabla f(x_{k+1}) - \alpha_k B_{k+1} d_k = \nabla f(x_k)$$

Which implies

$$\nabla(x_{k+1}) - \nabla f(x_k) = B_{k+1}(x_{k+1} - x_k)$$

This is the secant equation. We can use this equation to update B_{k+1} .

5.1.3 Trust Region Strategy

Problem 5.4 – Trust Region Strategy

Construct a model for f at x_k , $f(x_k + \Delta x) \sim mq(\Delta x) = f(x_k) + \Delta x^T \nabla f(x_k) + \frac{1}{2} \Delta x^T B_k \Delta x$, where $B_k \simeq \nabla^2 f(x_k)$. Construct region where we trust the model. Region can be a ball, eg. $\Omega_k = \{\Delta x \mid \|\Delta x\| \leq \delta_k^2\}$

The difference in trust region strategy and line search strategy is that in line search strategy, we first choose the direction, then choose step size. In trust region, we first choose the step size, then we choose the direction.

Definition 5.7 – Trust Region Strategy

In each iteration, we construct a model of f . That is, in each step we consider $m_k : \mathbb{R}^n \rightarrow \mathbb{R}$ that is a simple function that approximates f well on some simple set Ω_k (the trust region) around our current approximation x_k . Then we find the new approximation

$$\hat{x} = \operatorname{argmin}_{x \in \Omega_k} m_k(x)$$

A common model is the quadratic model

$$m_k(x) = f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \frac{1}{2} \langle x - x_k, B_k(x - x_k) \rangle$$

where $B_k \approx \nabla^2 f(x_k)$ approximates the Hessian. If the values $f(\hat{x})$ and $m_k(\hat{x})$ are close, then we declare $x_{k+1} = \hat{x}$. Otherwise, we shrink the size of the trust region Ω_k and repeat the process.

Usually Ω_k is a ball, ellipsoid, or a box around x_k .

The main points are how to choose a model function m_k , and how to choose a trust region Ω_k .

Definition 5.8 – Comparing Algorithms

[upload later](#)