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272284444

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# 1 Introduction

## 1.1 Lecture 1-Preliminaries

### Definition 1.1 – 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 1.1 – 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 1.2 – Classification of Quadratic Forms

Let  $Q$  be a quadratic form of a matrix  $A$ . Then  $Q$  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.
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.
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.
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.
5. indefinite if  $Q(x)$  can be positive or negative. Or there are positive and negative eigenvalues for  $A$ .

### Definition 1.3 – 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 1.4 – 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 1.5 – 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 1.6 – Chain Rule

WIP

### Definition 1.7 – 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  $\cos(\theta) = \frac{\langle x, y \rangle}{\|x\| \|y\|}$ .

With corresponding norm to be the Euclidean Norm

### Definition 1.8 – Open ball

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

### Definition 1.9 – map

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

### Definition 1.10 – open set

Let  $D \subset \mathbb{R}^n$ ,  $D$  open set.  $\forall x \in D, \exists \delta > 0$ , s.t  $B_\delta(x) \subset D$

**Definition 1.11 – 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 1.12 – 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  $f, g_i, h_i$  are all **affine** function and  $D = \mathbb{R}^2$ , then we have an LP

**Definition 1.13 – affine**

$$f(x) = Ax + b \tag{1}$$

where  $b \neq 0$

**Definition 1.14 – 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 1.15 – 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 1.16 – 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  $x \in I$ .

### Definition 1.17 – 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

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

## 1.2 Lecture 2

### Definition 1.18 – 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 1.2 – 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 1.19 – Contour

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

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

### Definition 1.20 – 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 1.21 – 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 1.3 – 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.

## 2 Unconstrained Optimization

### 2.1 Lecture 2

#### Problem 2.1 – 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

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

#### Theorem 2.1 – 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  $\Delta x$ .  $o(|\Delta x|)$ , the error term, means that the error goes to 0 faster than  $|\Delta x|$  as  $\Delta x$  goes to 0. Therefore, this is saying that the linear approximation becomes more and more accurate for smaller  $\Delta x$ .

**Definition 2.1 – Secant Line**

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

**Theorem 2.2 – 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 2.2 – 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

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

**Lemma 2.1 – 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  $\epsilon$  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 2.2 – 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 2.3**

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 2.3**

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

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

**Corollary 2.1 – Unconstrained optimality conditions on the real line**

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.* Omit here, can prove by using the little O or the definition

□

**Definition 2.3 – Hessian**



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

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

**Note:** The Hessian is always symmetric for  $C^2$  functions. We denote the vector space of symmetric matrices by  $S^n$ , we use the trace inner product for A,B symmetric matrices.  $\langle A, B \rangle = \text{trace} AB := \sum A_{i,j} B_{i,j}$

### Theorem 2.4 – 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  $\bar{x}$ .

### Lemma 2.2

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

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

## 2.2 Lecture 3

### Definition 2.4 – Matrix Norm

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

### Definition 2.5 – Multivariate unconstrained optimality conditions

Define  $f, D, \bar{x}$ ,  $D$  is an open set Then:

1. Nec: If  $\bar{x}$  is a local minimum for  $f$  on  $D$ , then  $\nabla f(\bar{x}) = 0$  and  $\nabla^2 f(\bar{x}) \succeq 0$  is positive semidefinite.
2. Suff: If  $\nabla f(\bar{x}) = 0$ ,  $\nabla^2 f(\bar{x}) \succ 0$  is positive definite then  $\bar{x}$  is a strict local minimum of  $f$  on  $D$ .

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

### Definition 2.6 – 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 2.4 – 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 2.5

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  $\epsilon d$ ? or  $d$  is the unit vector**

let  $d = -\nabla f(\bar{x}) / \|\nabla f(\bar{x})\|$  (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 2.7 – Cauchy’s method of steepest descent

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

$\|\nabla f(x_k)\| \approx 0$ ? If yes Stop

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

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

repeat

### Problem 2.6 – 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.

## 2.3 Lecture 4

### Problem 2.7 – How can we check if a matrix is positive definite/semidefinite

**Definition 2.8 – 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 2.9 – 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 2.1 – 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 2.10 – 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  $\lambda$  is called an **eigenvalue** of  $A$ .

**Theorem 2.5 – 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  $\lambda$ . 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 2.6 – 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 2.2**

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 2.2**

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 2.8 – 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 2.3 – Weierstrass Extreme Value Theorem**

If  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is continuous, and if  $D \subset \mathbb{R}^n$  is a closed and bounded set, then  $f$  is bounded below and the minimum value is attained on  $D$ .

**Definition 2.11 – 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 2.4 – Coercive Functions and Minimizers**

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

**Definition 2.12 – Level Sets**

Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  be a function and let  $\alpha \in \mathbb{R}$ . An  $\alpha$ -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 2.13 – Sub-level set**

Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  be a function and let  $\alpha \in \mathbb{R}$ . An  $\alpha$ -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 2.9**

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 2.5 – 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  $\lambda_i \geq 0$ ,  $\implies$  This part incomplete

□

**Theorem 2.7 – Weierstrass**

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

**Proposition 2.6**

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

*Proof.* Omit

□

**Theorem 2.8 –  $q(x)$  is coercive iff  $Q$  is positive definite**

*Proof.* Omit

□

### 3 Linear Least Squares & Solving Linear Systems

#### 3.1 Lecture 5

##### Problem 3.1 – 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 ( $\ell_1$  norm) is defined as

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

This can be formulated into a  $\ell_1$  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 3.1 – 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 3.1

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 3.2 – $\ell_1$ and $\ell_2$ Norm

The  $\ell_1$  norm of a vector  $x$  is defined to be

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

The  $\ell_2$  norm of a vector  $x$  is defined to be

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

### Problem 3.2 – Linear Least Squares Problem

Recall our  $\ell_1$  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  $\ell_2$  norm defined as  $\|e\|_2 = \sqrt{\sum e_i^2}$ . So our  $\ell_2$  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 3.3 – 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 3.4 – 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  $\sigma_{\max}$  be the largest singular value and  $\sigma_{\min}$  be the smallest singular value. Then

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

### Definition 3.5 – 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

## 3.2 Lecture 6

Goal: Solving normal equation/non linear case

### Definition 3.6 – 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  $A^T A$
- $\Sigma$  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 3.7 – Orthogonal Matrix**

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

**Definition 3.8 – 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).

**Definition 3.9 – QR Factorization**

For any  $m \times n$  matrix  $A$ , there exists an  $m \times m$  orthogonal matrix  $Q$  ( $Q Q^T = I$ ) 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 3.2 – 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  $A$ :

$$\begin{aligned} (A^T A)x &= A^T b \\ ((Q_1 R_1)^T Q_1 R_1)x &= (Q_1 R_1)^T b \\ (R_1^T Q_1^T Q_1 R_1)x &= R_1^T Q_1^T b \\ R_1^T R_1 x &= R_1^T Q_1^T b \\ R_1 x &= Q_1^T b \end{aligned}$$

Since  $Q_1$  is orthogonal

Since  $R_1$  is invertible

**Definition 3.10 – 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 3.3 – 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](#)

**Theorem 3.3 – 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  $\beta_k$  is chosen to ensure  $\langle Av_{k+1}, v_k \rangle = 0$ . This guarantees that the directions are  $A$ -conjugate **wtf is  $A$  conjugate**. We then set

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

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

**Problem 3.4**

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

- 1<sup>st</sup> & 2<sup>nd</sup> order optimality condition both necessary and sufficient
- 1<sup>st</sup>, 2<sup>nd</sup> order model

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

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

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

$$\begin{aligned} \min \frac{1}{2} \|Ax - b\|_2^2 &= f(x) \\ \text{s.t. } A &\in M_{m,n} \\ x &\in \mathbb{R}^n \end{aligned}$$

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

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

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

i.e., project  $b$  onto Range of  $A$

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

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  $\bar{x} + v, v \in \mathcal{N}(A)$  is a solution for all  $v$  in  $\mathcal{N}(A)$  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  $\mathcal{R}(A^T)$ .  
Given:

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

Where  $\Sigma$  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:

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

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:

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

For the solution  $B$ :

$$B\hat{x} = Bx = b + sb$$

Where:

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

### 3.3 Lecture 7

#### Definition 3.11 – 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 3.12 – 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 3.5 – 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  $\alpha$ .

### Definition 3.13 – 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  $f(x)$ .

## 4 Iterative Methods for Unconstrained Optimization

### 4.1 Lecture 8

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.

### Theorem 4.1 – Cauchy-Schwarz Inequality

Let  $x, y \in \mathbb{R}^n$ . Then

$$|\langle x, y \rangle| \leq \|x\| \|y\|$$

### Line Search Strategy

**Main Idea:** At a point  $x_k$ , we find the direction with the steepest descent (in the gradient direction) and move in that direction to a new point  $x_{k+1}$ .

**How do we choose step size?** We first set

$$g(\alpha) = f(x_k + \alpha \nabla f(x_k))$$

for step size  $\alpha$ , so we are traveling in the direction of the gradient (steepest descent). So now we have a one dimensional problem, then we can just solve for  $g'(\alpha) = 0$  to find the critical point in the direction of the gradient. After finding  $\alpha$ , we can obtain the next point  $x_{k+1} = x_k + \alpha \nabla f(x_k)$ .

### Definition 4.1 – Line Search Strategy

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

that approximately solves

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

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

#### Definition 4.2 – 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  $0 < \alpha < \bar{\alpha}$ .

#### Lemma 4.1

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

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

Then  $d$  is a descent direction for  $f$  at  $x$ .

### Trust Region Strategy

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 4.3 – 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  $\Omega_k$  (the trust region) around our current approximation  $x_k$ . Then we find the new approximation

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

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  $\Omega_k$  and repeat the process.

Usually  $\Omega_k$  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  $\Omega_k$ .

#### Problem 4.1 – 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  $f$ .

**Proposition 4.1**

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