

# Ch.4 Optimality Conditions

Review Calculus & Algebra

*PART - 2*

## ME511 – Principle of Optimum Design

Lecturer :

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# Introduction

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- In previous lecture we have discussed the optimality condition to check if the solution we get is optimum solution for single variable optimization.
- What if our optimization problem contain multiple design variables?
- In this case, it is important to know how to calculate **derivatives of functions** of several variables to solve optimization problems as well as to perform **matrix operation**

# Gradient of a Function

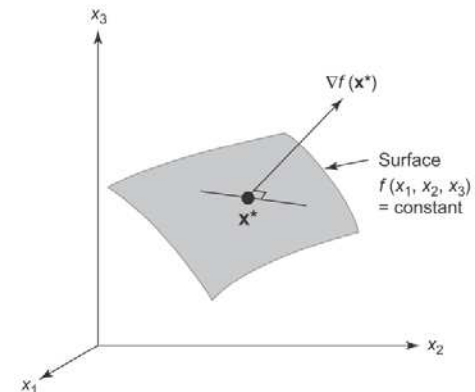
## First Partial Derivatives

For a function  $f(\mathbf{x})$  of  $n$  variables, the first partial derivatives are written as

$$\frac{\partial f(\mathbf{x})}{\partial x_i}; \quad i = 1 \text{ to } n$$

The  $n$  partial derivatives are usually arranged in a column vector known as the *gradient* of the function  $f(\mathbf{x})$ . The gradient is written as  $\partial f / \partial \mathbf{x}$  or  $\nabla f(\mathbf{x})$ . Therefore,

**Gradient**  $\rightarrow \mathbf{c} = \nabla f(\mathbf{x}) = \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \\ \vdots \\ \frac{\partial f(\mathbf{x})}{\partial x_n} \end{bmatrix}$

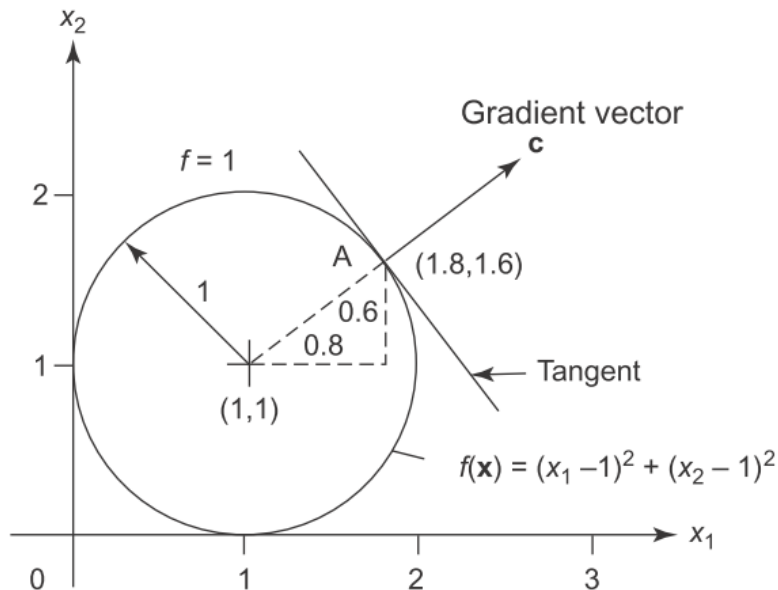


the gradient vector is normal to the tangent plane at the point  $\mathbf{x}$

# Gradient of a Function - Example

Calculate the gradient of  $f(\mathbf{x}) = (x_1 - 1)^2 + (x_2 - 1)^2$  at the point  $\mathbf{x}^* = (1.8, 1.6)$

For  $f(1.8, 1.6) = (1.8 - 1)^2 + (1.6 - 1)^2 = 1 \rightarrow$  a circle with center of (1,1) and radius of 1



$$\frac{\partial f}{\partial x_1}(1.8, 1.6) = 2(x_1 - 1) = 2(1.8 - 1) = 1.6$$

$$\frac{\partial f}{\partial x_2}(1.8, 1.6) = 2(x_2 - 1) = 2(1.6 - 1) = 1.2$$

$$\mathbf{c} = \begin{bmatrix} 1.6 \\ 1.2 \end{bmatrix} = [1.6 \quad 1.2]^T$$

# 2<sup>nd</sup> Derivatives of Functions –

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## *Second Partial Derivatives*

- If we differentiated again, we obtain second partial derivatives of  $f(\mathbf{x})$

$$\frac{\partial^2 f(\mathbf{x})}{\partial x_i \partial x_j}; \quad i, j = 1 \text{ to } n$$

- If we arrange them in matrix form, it is known as “**Hessian matrix**”, written as **H(x)**

$$\mathbf{H}(\mathbf{x}) = \nabla^2 f(\mathbf{x}) = \left[ \frac{\partial^2 f(\mathbf{x})}{\partial x_i \partial x_j} \right]_{n \times n}$$

# Hessian Matrix - Example

Derive with respect to  $x_2 \rightarrow$

For the following function, calculate the gradient vector and the Hessian matrix at the point (1, 2):

$$f(\mathbf{x}) = x_1^3 + x_2^3 + 2x_1^2 + 3x_2^2 - x_1x_2 + 2x_1 + 4x_2$$

## Solution

The first partial derivatives of the function are given as

$$\mathbf{c} = \nabla f(\mathbf{x}^*) = \begin{bmatrix} \frac{\partial f(\mathbf{x}^*)}{\partial x_1} \\ \frac{\partial f(\mathbf{x}^*)}{\partial x_2} \end{bmatrix}$$

$$\begin{aligned} \frac{\partial f}{\partial x_1} &= 3x_1^2 + 4x_1 - x_2 + 2 \\ \frac{\partial f}{\partial x_2} &= 3x_2^2 + 6x_2 - x_1 + 4 \end{aligned}$$

$$\mathbf{c} = \begin{bmatrix} 7 \\ 27 \end{bmatrix}$$

The second partial derivatives of the function are calculated by

$$\mathbf{H} \text{ or } \nabla^2 f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix}$$

$$\frac{\partial^2 f}{\partial x_1^2} = 6x_1 + 4; \quad \frac{\partial^2 f}{\partial x_1 \partial x_2} = -1;$$

$$\frac{\partial^2 f}{\partial x_2 \partial x_1} = -1; \quad \frac{\partial^2 f}{\partial x_2^2} = 6x_2 + 6.$$

$$\mathbf{H}(\mathbf{x}) = \begin{bmatrix} 6x_1 + 4 & -1 \\ -1 & 6x_2 + 6 \end{bmatrix}$$

The Hessian matrix at the point (1, 2)

$$\mathbf{H}(1, 2) = \begin{bmatrix} 10 & -1 \\ -1 & 18 \end{bmatrix}$$

# Eigenvalues

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- In optimization, it is necessary to calculate the *eigenvalues of Hessian matrix* to check if it satisfy the sufficient condition.
- If the eigenvalues are **positive definite** then the solution satisfy the sufficient condition for **minimum point**
- The eigenvalues can be found by solving the following:

$$|\mathbf{A} - \lambda \mathbf{I}| = 0 \quad : \text{where } \mathbf{A} \text{ is the Hessian Matrix}$$

*In order to do this we need to solve it using matrix operation*

# Taylor's Expansion

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- The idea of **Taylor's expansion** is fundamental to the development of optimum design and numerical methods
- A function can be approximated by polynomials of any point in terms of its **value** and **derivatives** using Taylor's expansion.

$$f(x) = f(x^*) + \frac{df(x^*)}{dx}(x - x^*) + \frac{1}{2} \frac{d^2f(x^*)}{dx^2}(x - x^*)^2 + R$$

1<sup>st</sup> derivative

2<sup>nd</sup> derivative

where  $R$  is the remainder term that is smaller in magnitude than the previous terms. It sometimes can be neglected if the value is insignificant



# Taylor's Expansion - Example

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Using Taylor expansion, approximate  $f(x) = \cos x$  around the point  $x^* = 0$

$$f(x) = f(x^*) + \frac{df(x^*)}{dx}(x - x^*) + \frac{1}{2} \frac{d^2f(x^*)}{dx^2}(x - x^*)^2 + R$$

## **Solution**

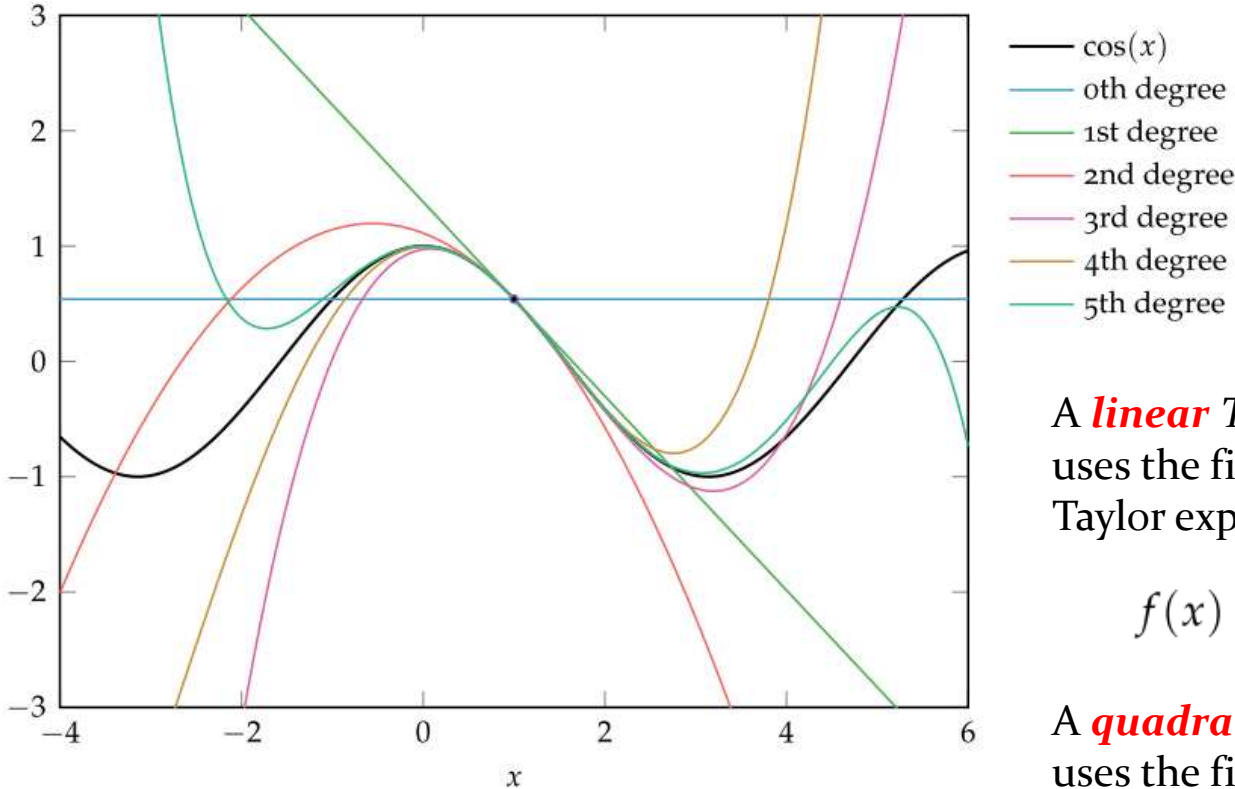
Derivatives of the function  $f(x)$  are given as

$$\frac{df}{dx} = -\sin x, \quad \frac{d^2f}{dx^2} = -\cos x$$

Therefore, the second-order Taylor's expansion for  $\cos x$  at the point  $x^* = 0$  is given as

$$\cos x \approx \cos 0 - \sin 0(x - 0) + \frac{1}{2}(-\cos 0)(x - 0)^2 = 1 - \frac{1}{2}x^2$$

# Taylor's Expansion - Example



$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!} (x - a)^n$$

A **linear** Taylor approximation uses the first two terms of the Taylor expansion

$$f(x) \approx f(a) + f'(a)(x - a)$$

A **quadratic** Taylor approximation uses the first three terms:

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

# Vector & Matrix Algebra

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- Consider this system of two simultaneous linear equations in three unknowns

$$\begin{aligned}x_1 + 2x_2 + 3x_3 &= 6 \\ -x_1 + 6x_2 - 2x_3 &= 3\end{aligned}$$

- We can represent above equations in the matrix form as

$$\begin{bmatrix} 1 & 2 & 3 \\ -1 & 6 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 6 \\ 3 \end{bmatrix} \quad \Rightarrow \quad \mathbf{Ax} = \mathbf{B}$$

Matrix A      Column Matrix B  
Vector  $\mathbf{x}$

# Matrix Operations

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- Let **A** and **B** are matrix of 2x2 below

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}$$

- Scaling with  $t \rightarrow t\mathbf{A} =$
- $\mathbf{A} + \mathbf{B} =$
- Multiplication (inner product)  $\rightarrow \mathbf{A}.\mathbf{B} =$
- Determinant of  $\mathbf{A} \rightarrow |\mathbf{A}| = a_{11}a_{22} - a_{12}a_{21}$
- Invers of  $\mathbf{A} \rightarrow \mathbf{A}^{-1} = \frac{1}{|\mathbf{A}|} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}$

**END OF THE SLIDES**