

• function in one variable

optimality conditions of

second order

↓

sufficient condition

for local extrema.

first order and

↓

necessary condition

for local extrema

• functions in several variables

$$f: T \rightarrow \mathbb{R},$$

$$T \subseteq \mathbb{R}^n, n > 1$$

$$f(x, y) = xy + x^2 \quad (\text{function in two variables})$$

Necessary Condition

$$f(x_1, x_2, \dots, x_n) = \text{diff } x_2,$$

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n} \right)$$

↓ diff w.r.t x_1 , considering all other variables x_2, \dots, x_n as constants

$(x_1^*, x_2^*, \dots, x_n^*)$ is a candidate for local maxima or minima

$$\text{If } \nabla f(x_1^*, x_2^*, \dots, x_n^*) = (0, \dots, 0)$$

Example:

$$f(x, y) = x - y + 2x^2 + 2xy + y^2$$

Example 1

$$f(x, y) = x - y + 2x^2 + 2xy + y^2$$

$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \right)$$

$$\nabla f = (1 + 4x + 2y, -1 + 2x + 2y)$$

$$\nabla f = (0, 0) \quad \parallel \quad (6, 0)$$

$$\begin{aligned} 1 + 4x + 2y &= 0 \\ -1 + 2x + 2y &= 0 \end{aligned}$$

$$\begin{pmatrix} 4x + 2y = -1 \\ 2x + 2y = 1 \end{pmatrix} \rightarrow x = -1, y = 3/2$$

$(-1, 3/2)$ is candidate for local maxima or local minima.

Hessian matrix of function $f(x, y)$

$$H_f(x, y) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} \quad \left(\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x} \right)$$

$$f(x, y) = x - y + 2x^2 + 2xy + y^2$$

$$\frac{\partial f}{\partial x} =$$

$$1 + 4x + 2y$$

$$\frac{\partial f}{\partial y} = -1 + 2x + 2y$$

$$\frac{\partial^2 f}{\partial x^2} =$$

$H_f(x, y) = \begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix}$

$\frac{\partial^2 f}{\partial x^2} = 4$
 $\frac{\partial^2 f}{\partial y \partial x} = 2$

$f(x_1, x_2, \dots, x_n)$

$H_f(x_1, x_2, \dots, x_n) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \dots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \dots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \dots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$

Row no. \downarrow $\frac{\partial^2 f}{\partial x_i \partial x_j}$ \downarrow Col. no.

Example $f(x, y, z) = x^2 + 2y^2 + 3z^2 + 2xy + 2xz$

$\frac{\partial f}{\partial x} = 2x + 2y + 2z$

$\frac{\partial f}{\partial y} = 4y + 2x$

$\frac{\partial f}{\partial z} = 6z + 2x$

$H_f(x, y, z) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial z \partial x} \\ 2 & 2 & 2 \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} & 0 \\ 2 & 0 & 6 \end{bmatrix}$

$\frac{\partial^2 f}{\partial y \partial x} = \frac{\partial^2 f}{\partial x \partial y}$ ✓

Symmetric matrix :-

$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}$

A be a matrix (square)

$$\begin{bmatrix} | & | & | \\ a_{11} & a_{12} & \dots & a_{1n} \\ | & | & | \end{bmatrix}$$
 A is called symmetric matrix if $a_{ij} = a_{ji}$

$\forall i, j$

i th row and j th column

j th row and i th column

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & \\ a_{31} & & a_{nn} \end{bmatrix}$$

$$\underline{\underline{A^t = A}}$$

Symmetric

Hessian matrix is always a symmetric matrix.

Positive (semi) definite matrix:- A symmetric matrix A is called positive (semi) definite matrix

if its all leading minors are positive. (Non-negative) \rightarrow zero + positive

n th leading minor
 = determinant of $n \times n$ submatrix in upper left corner

$$\begin{bmatrix} \boxed{a_{11}} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$n \times n$ matrix

\rightarrow total n leading minors.

$a_{11} \rightarrow$ first leading minor.

$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} \rightarrow$ second leading minor.

$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} \rightarrow$ third leading minor.

Example:- $\begin{bmatrix} 2 & 2 & 2 \\ 2 & 4 & 0 \\ & & \end{bmatrix}$

first leading minor = $2 > 0$
 second leading minor

✓

$$\begin{bmatrix} 2 & 4 & 0 \\ 2 & 0 & 6 \end{bmatrix}$$

second leading minor

$$\begin{vmatrix} 2 & 2 \\ 2 & 4 \end{vmatrix} = 8 - 4 = 4 > 0$$

Third leading minor

$$\begin{vmatrix} 2 & 4 & 0 \\ 2 & 0 & 6 \\ 2 & 0 & 6 \end{vmatrix} = 2 \begin{vmatrix} 4 & 0 \\ 0 & 6 \end{vmatrix} - 2 \begin{vmatrix} 2 & 0 \\ 2 & 6 \end{vmatrix} + 2 \begin{vmatrix} 2 & 4 \\ 2 & 0 \end{vmatrix}$$

$$= 2(24) - 2(12) + 2(-8) = 8 > 0$$

• This matrix is a positive definite matrix.

Negative semi-definite matrix :- k^{th} leading minor has sign $(-1)^k$, (or it is zero)

Example

$$\begin{pmatrix} -4 & 2 & 0 \\ 2 & -5 & 2 \\ 0 & 2 & -2 \end{pmatrix}$$

1st leading minor \rightarrow -ve
 second leading minor \rightarrow +ve
 third leading minor \rightarrow -ve
 } \rightarrow Negative definite matrix.

Sufficient Condition :- Let $f: D \rightarrow \mathbb{R}$ be multivariable function, $D \subseteq \mathbb{R}^n$.

A vector $X_0 \in D$ is local maxima if $\nabla f(X_0) = (0 \dots 0) \rightarrow (\alpha_1, \alpha_2, \dots, \alpha_n)$

① $\nabla^2 f(X_0)$
 ② Hessian matrix at X_0 is positive semi-definite. (Negative semi-definite)
 all minors must be Non-negative
 \Downarrow
 zero is positive.

- all numbers.

↓
zero is positive.

Convexity By Hessian matrix

Let $f: D \rightarrow \mathbb{R}$, $D \subseteq \mathbb{R}^n$ be a twice diff function on convex set D . If H_f is positive semi-definite for all x in D , then

f is a convex function in D .

- If H_f is a Negative semi-definite matrix $\forall x \in D$, then f is a concave function in D .

* Convex function

local minima
 \Rightarrow Global minima

* Concave function

local maxima
 \Rightarrow Global maxima.

Example :-

$$\begin{aligned} \text{Min } x^2 + y^2 + z^2 \\ \text{subject to } x^2 - z^2 = 1 \\ x^2 = z^2 + 1 \end{aligned}$$

$$* \text{ Min } (z^2 + 1) + y^2 + z^2$$

$$f(y, z) = y^2 + 2z^2 + 1$$

$$\nabla f(y, z) = \left(\frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right) = (2y, 4z)$$

$$\nabla f(y, z) = (0, 0) \quad \begin{aligned} y &= 0 \\ z &= 0 \end{aligned}$$

$(0, 0)$ is candidate local minima / local maxima

$$H_f = \begin{pmatrix} \frac{\partial^2 f}{\partial y^2} & \frac{\partial^2 f}{\partial y \partial z} \\ \frac{\partial^2 f}{\partial y \partial z} & \frac{\partial^2 f}{\partial z^2} \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix}$$

first leading minor = 2 > 0
 second leading minor = $\begin{vmatrix} 2 & 0 \\ 0 & 4 \end{vmatrix} = 8 > 0$
 positive ~~semi~~ definite matrix.

• $f(y, z)$ is a convex function

$$H_f|_{(0,0)} = \begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix} \text{ is also positive definite matrix}$$

$(0,0)$ is a local minimum

\Downarrow
 $(0,0)$ is a Global minimum

Line search method

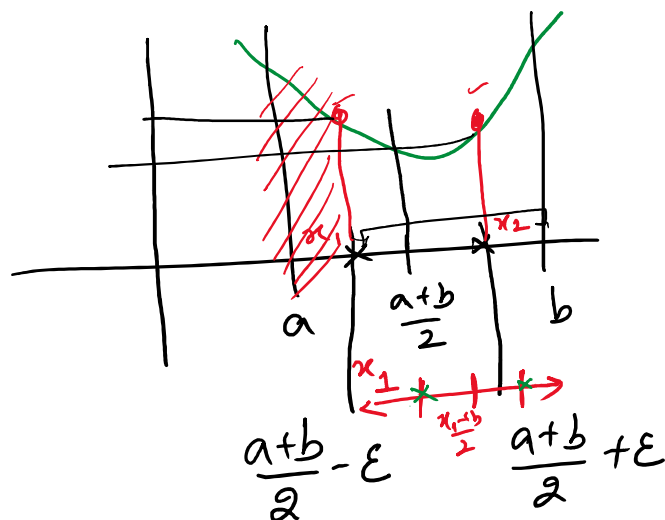
↙
 Golden section method

↘
 Fibonacci method

→ maxima or minima of single variable objective function in $[a, b]$

Unimodal in $[a, b]$:- The objective function $f(x)$ has only one local minima or local maxima (but not both) in this region $[a, b]$.

• Equal interval method



$f(x_1) < f(x_2)$?
 $f(x_1) > f(x_2)$?
 Yes

$$f(x_1) = f\left(\frac{a+b}{2} - \epsilon\right) \quad f\left(\frac{a+b}{2} + \epsilon\right) = f(x_2)$$

Golden section method → line search method
 function must be unimodal
 (only one

Golden Ratio \downarrow $\frac{0.618}{1} = g$
 local minima in interval of search)

Golden Ratio - 1

$$g = 0.618$$

Given $f(x) \rightarrow$ unimodal function in search interval $[a, b]$
 one local minima

$$g = 0.618$$

$$d = g(b-a)$$

$$x_1 = a + d, \text{ find } f(x_1) \text{ and } f(x_2)$$

$$x_2 = b - d$$

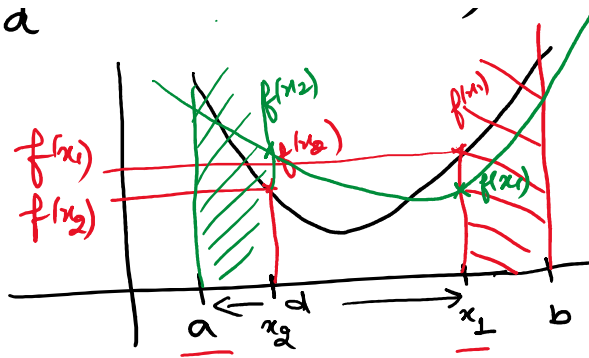
1 ✓ $f(x_1)$

2 ✓ $f(x_2)$

Yes
 $f(x_1) > f(x_2)$?

$f(x_1) < f(x_2)$?
 No

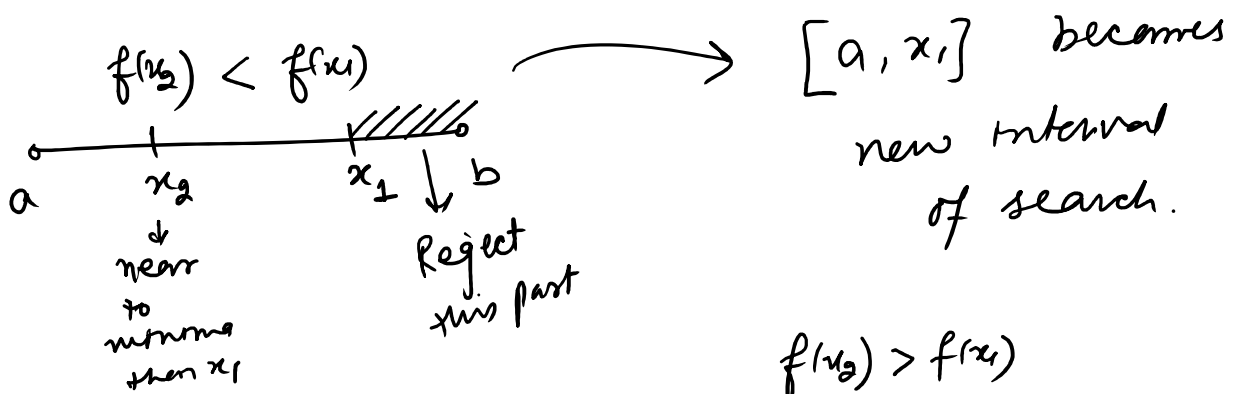
$$x_2 = b - a$$



$f(x_1) < f(x_2)$?
 Yes
 No

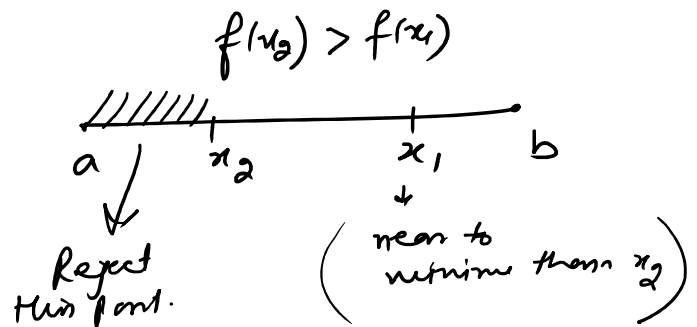
New interval of search becomes $[a, x_1]$

① $f(x_1) > f(x_2)$



② $f(x_1) < f(x_2)$

↓
 $[x_2, b]$ becomes new interval of search.



Example

$$f(x) = \underline{x^2 - 6x + 15}$$

min $f(x)$
 using G.S. method
 $[0, 4]$.

Hand calculation $a \rightarrow b$
 $\hookrightarrow [0, 10]$

$$g = 0.618 \sim 0.62$$

$$d = g(b - a) = 0.62 \times 10 = 6.2$$

$\therefore x_1 = 6.2$

$$d = g(b-a) = 0.62 \times 10 = 6.2$$

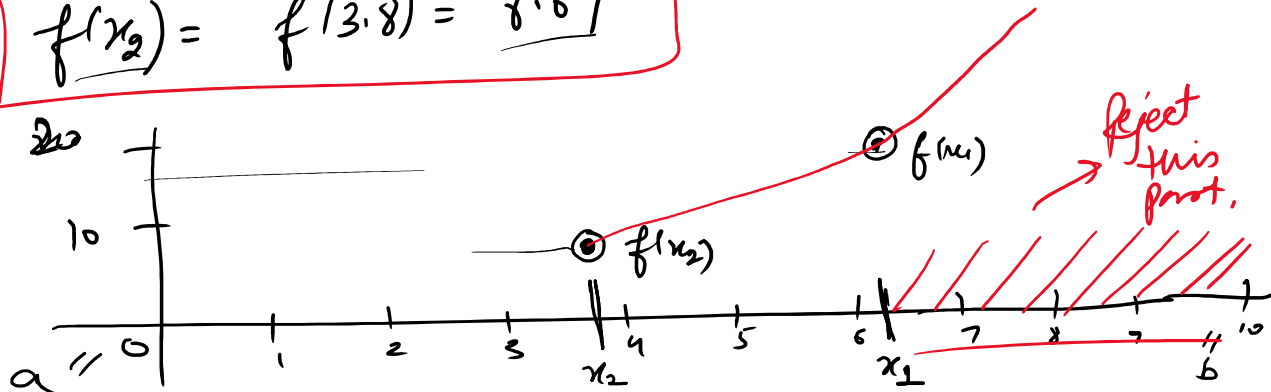
$$x_1 = a + d = 0 + 6.2 = 6.2$$

$$x_2 = b - d = 10 - 6.2 = 3.8$$

$$f(x_1) = f(6.2) = 16.24$$

$$f(x_1) > f(x_2)$$

$$f(x_2) = f(3.8) = 6.64$$



②

$$[a, x_1] = [0, 6.2]$$

$$g = 0.62$$

$$d = 0.62 \times (b-a) = 0.62 \times 6.2 = 3.8$$

$$x_1 = a + d = 0 + 3.8 = 3.8$$

$$x_2 = b - d = 6.2 - 3.8 = 2.4$$

$$f(x_1) = f(3.8) = 6.64$$

$$f(x_2) = f(2.4) =$$

By algorithm
of Golden
section

