INDIAN INSTITUTE OF SCIENCE

Water Resources Systems:
Modeling Techniques and Analysis

Lecture - 4

Course Instructor : Prof. P. P. MUJUMDAR
Department of Civil Engg., IISc.

Summary of the previous lecture

- Optimization and simulation
- Optimization: Methods of Calculus
  - Function of a single variable
    - Local maximum, Local minimum
    - Saddle point
    - Global maximum, Global minimum
    - Convex, Concave functions

Optimization: Methods of Calculus

$f(x)$: function of a single variable

The necessary condition:

At a local optimum (maximum or minimum),

$$f'(x) = 0$$

$x = x_0$ …………. Stationary point

Sufficiency condition

$$f''(x)\Big|_{x_0} < 0 \qquad \ldots \qquad \text{maximum}$$

$$f''(x)\Big|_{x_0} > 0 \qquad \ldots \qquad \text{minimum}$$

Optimization: Methods of Calculus

If $\frac{d^2 f}{dx^2} = 0$

Find the first higher order non-zero derivative; let this be n^{th} order derivative,

$$\left.\begin{aligned} \frac{df}{dx} = \frac{d^2 f}{dx^2} = \frac{d^3 f}{dx^3} = \ldots\ldots \frac{d^{n-1} f}{dx^{n-1}} = 0 \\ \frac{d^n f}{dx^n} \neq 0 \end{aligned}\right\}$$

at the stationary point, $x = x_0$

Optimization: Methods of Calculus

- If n is even and
  - if $\left.\dfrac{d^n f}{dx^n}\right|_{x_0} > 0$, x_0 is a local minimum
  - if $\left.\dfrac{d^n f}{dx^n}\right|_{x_0} < 0$, x_0 is a local maximum
- If n is odd, x_0 is a saddle point (neither a minimum nor a maximum)

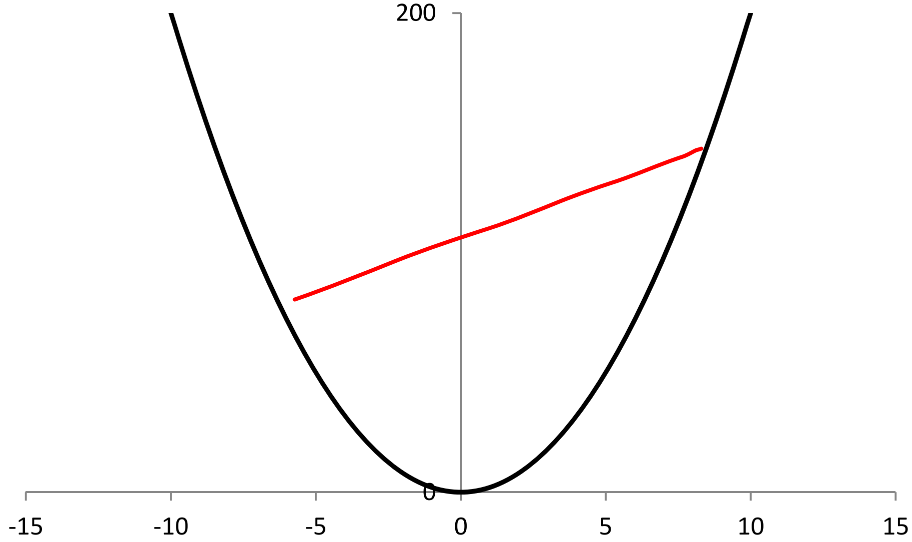
Example – 1

Convex function:

$$f\left(x\right) = 2x^2$$

$$\frac{df}{dx} = 4x$$

$$\frac{d^2 f}{dx^2} = 4 \quad > \quad 0$$



For a convex function,

$$f\left[\alpha x_1 + \left(1-\alpha\right) x_2\right] < \alpha f\left(x_1\right) + \left(1-\alpha\right) f\left(x_2\right)$$

Example – 1 (Contd.)

$$x_1 = 0;\; x_2 = 2 \qquad \alpha = 0.5$$

LHS $= f\left[\alpha x_1 + (1-\alpha) x_2\right]$

$= f\left[0 + 0.5 * 2\right]$

$= f\left[1\right]$

$= 2$

RHS $= \alpha f(x_1) + (1-\alpha) f(x_2)$

$= 0.5 \times f(0) + 0.5 \times f(2)$

$= 0.5 \times 0 + 0.5 \times 2 \times 4$

$= 4$

LHS < RHS

i.e., $f\left[\alpha x_1 + (1-\alpha) x_2\right] < \alpha f(x_1) + (1-\alpha) f(x_2)$

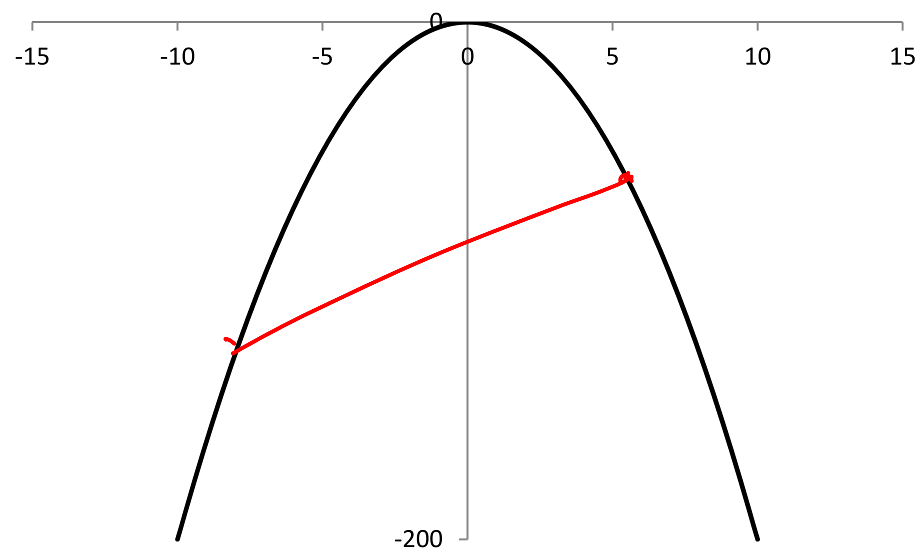
Example – 1 (Contd.)

Concave function:

$$f(x) = -2x^2$$

$$\frac{df}{dx} = -4x$$

$$\frac{d^2 f}{dx^2} = -4 \quad < \quad 0$$



For a concave function,

$$f\left[\alpha x_1 + (1-\alpha) x_2\right] > \alpha f(x_1) + (1-\alpha) f(x_2)$$

Example – 2

Check for optimal values of

$$f(x) = 3x^3 - 6x^2 + 4x - 7$$

$$f^{'}(x) = 9x^2 - 12x + 4$$

$$f^{'}(x) = 0$$

$$9x^2 - 12x + 4 = 0$$

$$x_0 = \frac{12 \pm \sqrt{144 - 4 \times 9 \times 4}}{2 \times 9} = \frac{2}{3}$$

Only one solution exists

Example – 2 (Contd.)

$$f'(x) = 9x^2 - 12x + 4$$

$$f''(x) = 18x - 12$$

$$f''(x)\Big|_{x_0} = 18 \times \frac{2}{3} - 12 = 0$$

Looking for next higher derivatives

$$f'''(x) = 18 \neq 0$$

As n (= 3) is odd, the function $f(x)$ is neither a minimum nor a maximum at $x_0 = 2/3$

Example – 3

Check for optimal values of

$$f\left(x\right)=12x^5-15x^4-40x^3+81$$

$$f^{'}\left(x\right)=60x^4-60x^3-120x^2$$

$$f^{'}\left(x\right)=0$$

$$60x^4-60x^3-120x^2=0$$

$$60x^2\left(x+1\right)\left(x-2\right)=0$$

$x=0,\ \ x=-1$ and $x=2$

Example – 3 (Contd.)

$$f^{'}\left(x\right)=60x^4-60x^3-120x^2$$

$$f^{''}\left(x\right)=240x^3-180x^2-240x$$

$$f^{''}\left(x\right)\Big|_{x=0}=0$$

$$f^{'''}\left(x\right)=720x^2-360x-240$$

$$f^{'''}\left(x\right)\Big|_{x=0}=240\neq 0$$

Neither a minimum nor a maximum exists at $x=0$

Example – 3 (Contd.)

$$f''(x) = 240x^3 - 180x^2 - 240x$$

$$f''(x)\Big|_{x=-1} = -180$$ -ve value

Therefore maximum occurs at $x = -1$

$$f(x) = 12x^5 - 15x^4 - 40x^3 + 81$$

$$= 94$$

Example – 3 (Contd.)

$$f''(x) = 240x^3 - 180x^2 - 240x$$

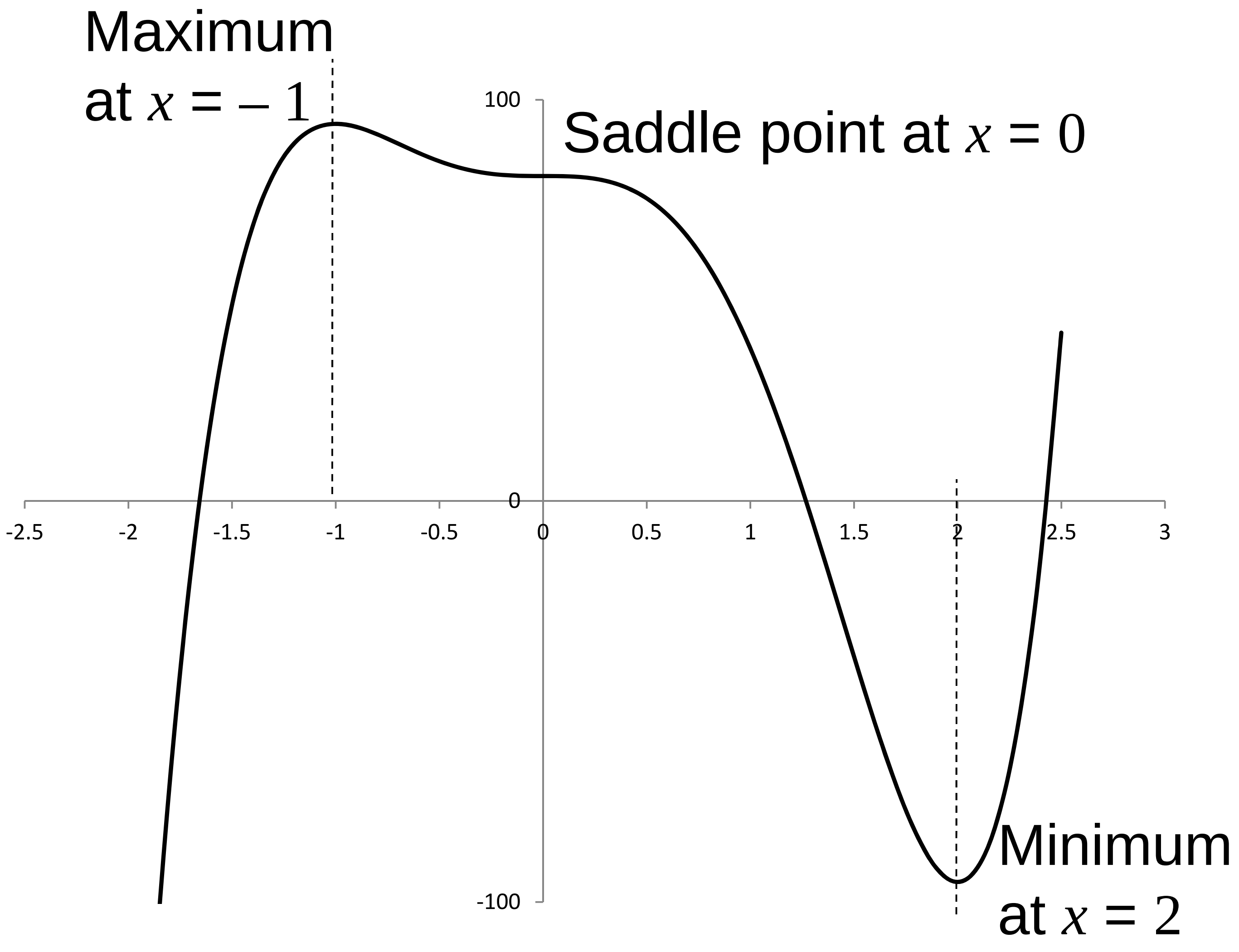
$$f''(x)\Big|_{x=2} = 720$$ +ve value

Therefore minimum occurs at $x = 2$

$$f(x) = 12x^5 - 15x^4 - 40x^3 + 81$$

$$= -95$$

Example – 3 (Contd.)



Optimization: Methods of Calculus

Function of multiple variables:

- $f(X)$ is a function of n variables represented by vector $X = (x_1, x_2, x_3, \ldots\ldots x_n)$

- Necessary condition for stationary point $X = X_0$ is, each first partial derivative of $f(X)$ should be zero.

$$\frac{\partial f}{\partial x_1} = \frac{\partial f}{\partial x_2} = \ldots\ldots\ldots = \frac{\partial f}{\partial x_n} = 0$$

Optimization: Methods of Calculus

- $H[f(X)]$ is Hessian matrix of function $f(X)$
- Hessian matrix is defined as

$$H\left[f(X)\right]= \begin{array}{c} \\ x_1 \\ x_2 \\ . \\ . \\ . \\ x_n \end{array} \begin{array}{c} \begin{array}{cccc} x_1 & x_2 & \ldots. & x_n \end{array} \\ \begin{bmatrix} \dfrac{\partial^2 f(X)}{\partial x_1^2} & \dfrac{\partial^2 f(X)}{\partial x_1 \partial x_2} & .... & \dfrac{\partial^2 f(X)}{\partial x_1 \partial x_n} \\ \dfrac{\partial^2 f(X)}{\partial x_2 \partial x_1} & \dfrac{\partial^2 f(X)}{\partial x_2^2} & .... & \dfrac{\partial^2 f(X)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & & \vdots \\ \dfrac{\partial^2 f(X)}{\partial x_n \partial x_1} & \dfrac{\partial^2 f(X)}{\partial x_n \partial x_2} & .... & \dfrac{\partial^2 f(X)}{\partial x_n^2} \end{bmatrix} \end{array}$$

Optimization: Methods of Calculus

- Sufficiency condition:
  - H positive definite at $X = X_0$ … ~~Maximum~~ Minimum
  - H negative definite at $X = X_0$ …. ~~Minimum~~ Maximum

- A square matrix is positive definite if all the eigen values are positive.
- A square matrix is negative definite if all the eigen values are negative.

Optimization: Methods of Calculus

- The eigen values (λ) of Hessian matrix are given by roots of characteristic equation

$$\left|\lambda I - H\right| = 0$$

I is identity matrix.

Optimization: Methods of Calculus

- If all the eigen values of Hessian matrix are positive, then the function is strictly convex.

- If all the eigen values of Hessian matrix are negative, then the function is strictly concave.

- If some eigen values are positive and some are negative or if some are zero, then the function is neither strictly convex nor strictly concave.

Optimization: Methods of Calculus

Whether the function is minimum or maximum at $X = X_0$ depends on nature of eigen values of its Hessian matrix evaluated at X_0 .

1. If all eigen values are positive at X_0, X_0 is a local minimum. If all eigen values are positive for all possible values of X, then X_0 is a global minimum.
2. If all eigen values are negative at X_0, X_0 is a local maximum. If all eigen values are negative for all possible values of X, then X_0 is a global maximum.
3. If some eigen values are positive and some are negative or some are zero, then X_0 is neither a local minimum nor a local maximum.

Example – 4

Examine the function for convexity/concavity and determine the values at extreme points

$$f\left(X\right) = x_1^2 + x_2^2 - 4x_1 - 2x_2 + 5$$

The stationary point is obtained by solving

$$\frac{\partial f}{\partial x_1} = 2x_1 - 4 = 0 \qquad \text{and} \qquad \frac{\partial f}{\partial x_2} = 2x_2 - 2 = 0$$

$$x_1 = 2,\ x_2 = 1$$

$$X = \left(2,1\right)$$

Example – 4 (Contd.)

- Hessian matrix is

$$H\left[f(X)\right]=\begin{bmatrix}\dfrac{\partial^2 f(X)}{\partial x_1^2} & \dfrac{\partial^2 f(X)}{\partial x_1 \partial x_2}\\ \dfrac{\partial^2 f(X)}{\partial x_2 \partial x_1} & \dfrac{\partial^2 f(X)}{\partial x_2^2}\end{bmatrix}_{(2,1)}$$

Hessian matrix evaluated at stationary point (2,1)

Example – 4 (Contd.)

$$f\left(X\right)=x_1^2+x_2^2-4x_1-2x_2+5$$

$$\frac{\partial f}{\partial x_1}=2x_1-4 \qquad \frac{\partial^2 f}{\partial x_1 \partial x_2}=0$$

$$\frac{\partial^2 f}{\partial x_1^2}=2$$

$$\frac{\partial f}{\partial x_2}=2x_2-2 \qquad \frac{\partial^2 f}{\partial x_2 \partial x_1}=0$$

$$\frac{\partial^2 f}{\partial x_2^2}=2$$

Example – 4 (Contd.)

Hessian matrix is

$$H\left[f\left(X\right)\right]=\begin{bmatrix}2 & 0\\0 & 2\end{bmatrix}$$

Eigen values of Hessian matrix:

$$\left|\lambda I-H\left[f\left(X\right)\right]\right|=0$$

$$\left|\lambda I-H\right|=\begin{vmatrix}\lambda-2 & 0\\0 & \lambda-2\end{vmatrix}=0$$

$$\left(\lambda-2\right)^2=0$$

Eigen values are $\lambda_1=2,\ \lambda_2=2$

Example – 4 (Contd.)

- As both the eigen values are positive, the matrix is positive definite

Hence the function has local minimum at $X = (2,1)$

As the Hessain matrix does not depend on x_1 and x_2 and it is positive definite matrix, the function is strictly convex and therefore the local minimum is also the global minimum