INDIAN INSTITUTE OF SCIENCE

Water Resources Systems:

Modeling Techniques and Analysis

Lecture - 5

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Summary of the previous lecture

- Optimization of a function of a single variable

  necessary condition $f'(x) = 0$

  Sufficiency condition $f''(x)\Big|_{x_0} < 0$ $\quad f''(x)\Big|_{x_0} > 0$

Function of multiple variables

necessary condition $$\frac{\partial f}{\partial x_1} = \frac{\partial f}{\partial x_2} = \dots\dots\dots = \frac{\partial f}{\partial x_n} = 0$$

Sufficiency condition:

Hessian matrix $$H\left[f(X)\right] = \begin{bmatrix} \frac{\partial^2 f(X)}{\partial x_1^2} & \frac{\partial^2 f(X)}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f(X)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(X)}{\partial x_2^2} \end{bmatrix}$$

- H positive definite at X = X_0 … Minimum
- H negative definite at X = X_0 …. Maximum

Example – 1

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

$$f(X) = -x_1^2 - x_2^2 - 4x_1 - 8$$

The stationary point is obtained by solving

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

$$x_1 = -2,\ x_2 = 0$$

$$X = (-2, 0)$$

Example – 1 (Contd.)

- Hessian matrix is

$$H\left[f\left(X\right)\right]=\begin{bmatrix}\dfrac{\partial^2 f\left(X\right)}{\partial x_1^2} & \dfrac{\partial^2 f\left(X\right)}{\partial x_1\partial x_2}\\ \dfrac{\partial^2 f\left(X\right)}{\partial x_2\partial x_1} & \dfrac{\partial^2 f\left(X\right)}{\partial x_2^2}\end{bmatrix}_{\left(-2,0\right)}$$

Hessian matrix evaluated at stationary point (-2,0)

Example – 1 (Contd.)

$$f\left(X\right) = -x_1^2 - x_2^2 - 4x_1 - 8$$

$$\begin{bmatrix} \dfrac{\partial^2 f\left(X\right)}{\partial x_1^2} & \dfrac{\partial^2 f\left(X\right)}{\partial x_1 \partial x_2} \\ \dfrac{\partial^2 f\left(X\right)}{\partial x_2 \partial x_1} & \dfrac{\partial^2 f\left(X\right)}{\partial x_2^2} \end{bmatrix}$$

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

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

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

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

Example – 1 (Contd.)

Hessian matrix is

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

Eigen values of Hessian matrix:

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

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

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

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

Example – 1 (Contd.)

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

Hence the function has local maximum at $X = \left(-2, 0\right)$

As the Hessain matrix does not depend on x_1 and x_2 and it is negative definite matrix, the function is strictly concave and therefore the local maximum is also the global maximum

Example – 2

Determine the extreme values of the function

$$f\left(X\right) = x_1^3 + x_2^3 - 3x_1 - 12x_2 + 20$$

The stationary point is obtained by solving

$$\frac{\partial f}{\partial x_1} = 3x_1^2 - 3 = 0 \qquad x_1 = \pm 1$$

and

$$\frac{\partial f}{\partial x_2} = 3x_2^2 - 12 = 0 \qquad x_2 = \pm 2$$

Four solutions

$X = \left(-1,-2\right), \quad \left(1,2\right), \quad \left(1,-2\right)$ and $\left(-1,2\right)$

Example – 2 (Contd.)

- Hessian matrix is

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

$$f\left(X\right)=x_1^3+x_2^3-3x_1-12x_2+20$$

$$\frac{\partial f}{\partial x_1}=3x_1^2-3 \qquad \frac{\partial^2 f}{\partial x_1 \partial x_2}=0$$

$$\frac{\partial^2 f}{\partial x_1^2}=6x_1$$

Example – 2 (Contd.)

$$f\left(X\right)=x_1^3+x_2^3-3x_1-12x_2+20$$

$$\frac{\partial f}{\partial x_2}=3x_2^2-12 \qquad \frac{\partial^2 f}{\partial x_2 \partial x_1}=0$$

$$\frac{\partial^2 f}{\partial x_2^2}=6x_2$$

Hessian matrix is

$$H\left[f\left(X\right)\right]=\begin{bmatrix} 6x_1 & 0 \\ 0 & 6x_2 \end{bmatrix}$$

Example – 2 (Contd.)

Hessian matrix is

$$H\left[f\left(X\right)\right]=\begin{bmatrix}6x_1 & 0\\ 0 & 6x_2\end{bmatrix}$$

Eigen values of Hessian matrix:

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

$$\left|\lambda I-H\right|=\begin{bmatrix}\lambda-6x_1 & 0\\ 0 & \lambda-6x_2\end{bmatrix} = 0$$

$$\left(\lambda-6x_1\right)\left(\lambda-6x_2\right)=0$$

Eigen values are $\lambda_1=6x_1,\ \lambda_2=6x_2$

Example – 2 (Contd.)

Hessian matrix at

$$H\left[f\left(X\right)\right]=\begin{bmatrix}6x_1 & 0\\ 0 & 6x_2\end{bmatrix}_{(1,2)}$$

Eigen values are $\lambda_1 = 6x_1,\ \lambda_2 = 6x_2$

$$\lambda_1 = 6,\ \lambda_2 = 12$$

All the eigen values of Hessian matrix are positive, hence the matrix is positive definite at $X = (1,2)$

Therefore the function has a local minimum at this point

$$f_{\min}\left(X\right) = 1^3 + 2^3 - 3\times 1 - 12\times 2 + 20 = 2$$

Example – 2 (Contd.)

Hessian matrix at

$$H\left[f\left(X\right)\right]=\begin{bmatrix}6x_1 & 0\\ 0 & 6x_2\end{bmatrix}_{\left(-1,-2\right)}$$

Eigen values are $\lambda_1 = 6x_1,\ \lambda_2 = 6x_2$

$$\lambda_1 = -6,\ \lambda_2 = -12$$

All the eigen values of Hessian matrix are negative, hence the matrix is negative definite at $X = \left(-1,-2\right)$

Therefore the function has a local maximum at this point

$$f_{\max}\left(X\right)=\left(-1\right)^3+\left(-2\right)^3-3\times\left(-1\right)-12\times\left(-2\right)+20$$

$$=38$$

Example – 2 (Contd.)

Hessian matrix at

$$H\left[f\left(X\right)\right]=\begin{bmatrix}6x_1 & 0\\ 0 & 6x_2\end{bmatrix}_{\left(-1,2\right)\ or\ \left(1,-2\right)}$$

Eigen values are -6 and 12 (or 6 and -12)

The H matrix is neither positive definite nor negative definite at these two points

Constrained Optimization

Optimization: Methods of Calculus

Constrained Optimization:

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

Maximize or Minimize $f(X)$

Subject to (s.t.) $g_j(X) \leq 0$ $\qquad j = 1, 2, \ldots.. m$

$m \leq n$

$f(X)$ and $g(X)$ may or may not be linear functions

- If $m > n$ the problem is over defined and there will be no solution unless redundant constrains are present

Optimization: Methods of Calculus

Constrained Optimization:

- Function with equality constraints
- Function with inequality constraints

Function with equality constraints

Maximize or Minimize $f(X)$

(s.t.) $g_j(X) = 0$ $\quad j = 1, 2, \ldots m$

$$X = \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{Bmatrix}$$

Two methods discussed

- Direct substitution
- Lagrange multipliers

Optimization: Methods of Calculus

Direct substitution:

- Reduce the problem to an unconstrained problem by expressing m variables in terms of the remaining $(n - m)$ variables.

For example,

3 variables : x_1, x_2, x_3

2 constraints

x_2, x_3 may be expressed in terms of x_1 and render the problem as unconstrained problem with only x_1 involved

Optimization: Methods of Calculus

Limitation:

- With higher no. of variables and constraints this method becomes quite cumbersome.
- Constraint equations are often non-linear – difficult to solve them simultaneously.

Example – 3

Minimize the function

$$f\left(X\right)=x_1^2+x_2^2+4x_1x_2$$

s.t.

$$x_1+x_2-4=0$$

Solution:

$$x_1=4-x_2$$

The modified function is

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

$$=16+8x_2-2x_2^2$$

Example – 3 (Contd.)

$$\frac{\partial f}{\partial x_2} = 8 - 4x_2$$

$$\frac{\partial f}{\partial x_2} = 0$$

$$8 - 4x_2 = 0$$

$$x_2 = 2$$

$$\frac{\partial^2 f}{\partial x_2^2} = -4 \quad < 0,$$

Local

~~Global~~ maximum occurs at $x_2 = 2$

Optimization: Methods of Calculus

Lagrange multipliers:

Maximize or Minimize $f(X)$

s.t.

$g_j(X) = 0 \qquad j = 1, 2, \ldots.. m$

- Introduce one additional variable corresponding to each constraint.
- Lagrange function $\cancel{f(X)}$ is written as

$$\cancel{L = f(X) - \lambda_j g_j(X)} \qquad L = f(x) - \sum_{j=1}^{m} \lambda_j g_j(x)$$

- When $g_j(X) = 0$, optimizing L is same as optimizing $f(X)$
- The problem is transformed to unconstrained optimization problem

Optimization: Methods of Calculus

$$L = f\left(X\right) - \lambda_1 g_1\left(X\right) - \lambda_2 g_2\left(X\right) - \ldots\ldots - \lambda_m g_m\left(X\right)$$

- The problem of n variables with m constraints is changed to a single problem of $(n+m)$ variables with no constraints.

Optimization: Methods of Calculus

Necessary condition: For a function $f(X)$ subject to the constraints $g_j(X)$ =0, $j = 1, 2, \ldots.. m$ to have a relative optimum at a point X^* is that the first partial derivatives of the Langrange function with respect to each of its arguments must be zero.

$$L = f\left(X\right) - \sum_{j=1}^{m} \lambda_j g_j\left(X\right)$$

$$\frac{\partial L}{\partial x_i} = 0 \qquad i = 1, 2, \ldots.. n$$

$$\frac{\partial L}{\partial \lambda_j} = 0 \qquad j = 1, 2, \ldots.. m$$

Optimization using Calculus

The $(n + m)$ simultaneous equations are solved to get a solution, (X^*, λ^*) .

Sufficiency condition:

The second partial derivatives are denoted by

$$L_{ij} = \left. \frac{\partial^2 L}{\partial x_i \partial x_j} \right|_{(X^*, \lambda^*)} \qquad i = 1, 2, \ldots.. n$$

$$g_{ij} = \left. \frac{\partial g_j(X)}{\partial x_i} \right|_{X^*} \qquad j = 1, 2, \ldots.. m$$

Optimization using Calculus

Sufficiency condition:

$$
|D| = \begin{array}{r|cccc:cccc|}
 & \multicolumn{4}{c}{\overbrace{\qquad\qquad\qquad\qquad\qquad\qquad}^{n\text{ terms}}} & \multicolumn{4}{c}{\overbrace{\qquad\qquad\qquad\qquad}^{m\text{ terms}}} \\
\left.\begin{array}{r} \\ \\ n \\ \text{terms} \\ \\ \end{array}\right\{ &
\begin{array}{c} L_{11}-Z \\ L_{21} \\ . \\ . \\ L_{n1} \end{array} &
\begin{array}{c} L_{12} \\ L_{22}-Z \\ . \\ . \\ L_{n2} \end{array} &
\begin{array}{c} .... \\ .... \\ \\ \\ .... \end{array} &
\begin{array}{c} L_{1n} \\ L_{2n} \\ . \\ . \\ L_{nn}-Z \end{array} &
\begin{array}{c} g_{11} \\ g_{12} \\ . \\ . \\ g_{1n} \end{array} &
\begin{array}{c} g_{21} \\ g_{22} \\ . \\ . \\ g_{2n} \end{array} &
\begin{array}{c} ... \\ ... \\ \\ \\ ... \end{array} &
\begin{array}{c} g_{m1} \\ g_{m2} \\ . \\ . \\ g_{mn} \end{array} \\
\hdashline
\left.\begin{array}{r} \\ \\ m \\ \text{terms} \\ \\ \end{array}\right\{ &
\begin{array}{c} g_{11} \\ g_{21} \\ . \\ . \\ g_{m1} \end{array} &
\begin{array}{c} g_{12} \\ g_{22} \\ . \\ . \\ g_{m2} \end{array} &
\begin{array}{c} .... \\ .... \\ \\ \\ .... \end{array} &
\begin{array}{c} g_{1n} \\ g_{2n} \\ . \\ . \\ g_{mn} \end{array} &
\begin{array}{c} 0 \\ 0 \\ . \\ . \\ 0 \end{array} &
\begin{array}{c} 0 \\ 0 \\ . \\ . \\ 0 \end{array} &
\begin{array}{c} ... \\ ... \\ . \\ . \\ ... \end{array} &
\begin{array}{c} 0 \\ 0 \\ . \\ . \\ 0 \end{array}
\end{array}
$$

$$|D| = 0$$

Optimization using Calculus

Leads to a polynomial in Z of the order $(n - m)$

Solve for Z

If all Z values are positive ….. X* corresponds to minimum

If all Z values are negative ….. X* corresponds to maximum

If some values are positive and some are negative … X* is neither a minimum nor a maximum.