IIT KHARAGPUR

NPTEL ONLINE CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Basic Concepts of Optimization – II

(WEEK – 4: LECTURE – 16)

Dr. Debasis Sarkar

Department of Chemical Engineering

Indian Institute of Technology Kharagpur

Basic Concepts of Optimization – II

Week 4:

- Equality constrained problems: Introduction
- Variable elimination method
- Method of constrained variation
- Lagrange multipliers
- General Nonlinear Programming Problems
- Kuhn Tucker conditions

Today's Topic:

- Equality constrained problems
- Variable elimination method
- Method of constrained variation

Unconstrained Vs Constrained Problems

Unconstrained optimization finds the minimum of a function under the assumption that the decision variables can take on any possible value.

But generally, additional constraints exist that limit the range of feasible values for decision variables.

$$\min_x f(x) \text{ s.t. } x \in B$$

$\min_x f(x)$

What is the minimum for $f(x) = (x-4)^2$?

Answer: $x = 4$

What is the minimum for $f(x) = (x-4)^2$ subject to $x \geq 5$

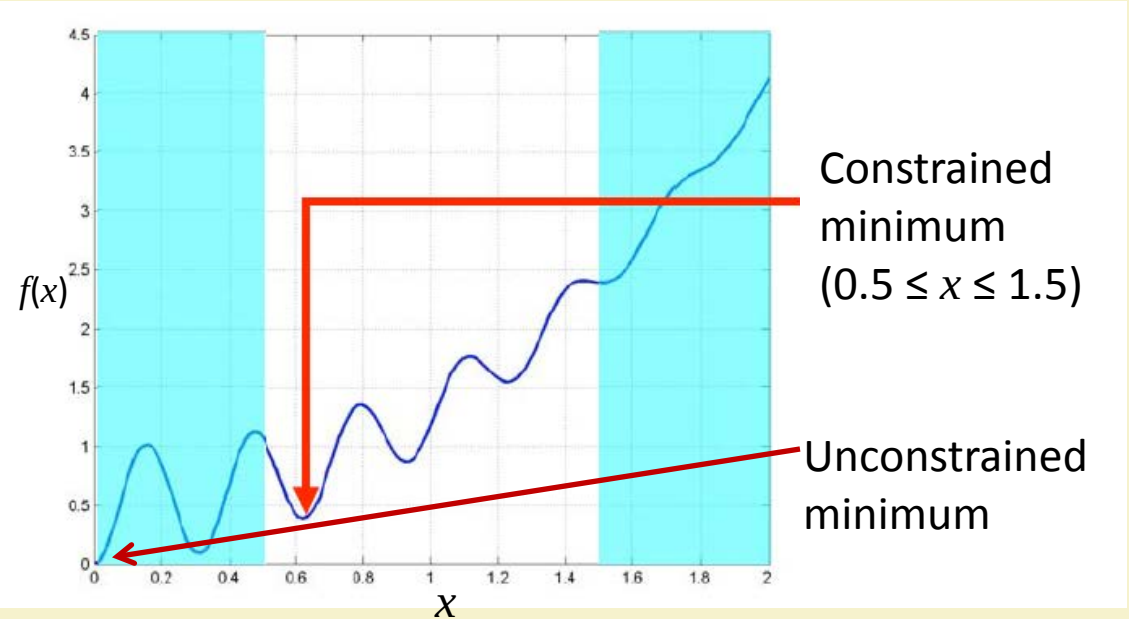
Answer: 5

Note that $x = 5$ is not a stationary point for unconstrained problem.

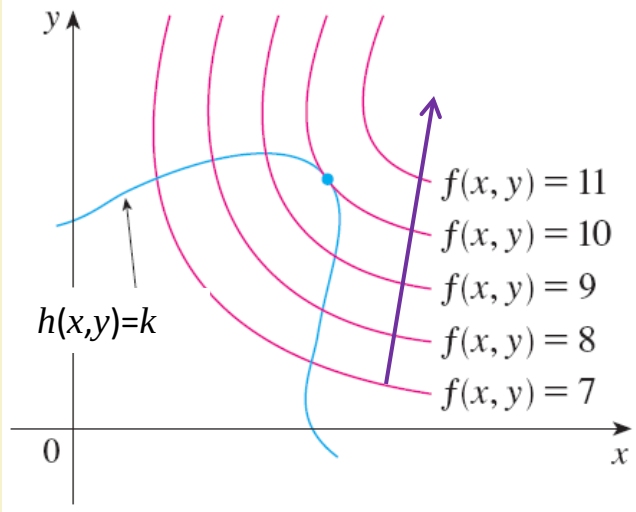
$f'(5) = 2(x - 4)|_{x=5} = 2$

Unconstrained Vs Constrained Problems

Find Minimum



Find Maximum



Equality Constrained Problems: Problem Statement

Problem Statement:

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{x}) \\ \text{subject to:} \quad & h_i(\mathbf{x}) = 0 \; \forall i = 1, 2, \ldots m \\ & \mathbf{x} \in \mathbb{R}^n \end{aligned}$$

or

$$\min_{\mathbf{x}} f(\mathbf{x}) \quad \text{subject to} \quad \mathbf{h}(\mathbf{x}) = 0$$

$$\mathrm{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

Note that $m \leq n$. If $m > n$, then the problem will be over-defined and there will be no solution.

The function of multiple variables, $f(x)$, may be subject to one or more equality constraints of many variables. These equality constraints may or may not be linear.

Equality Constrained Problems: Method of Solution

1. Variable elimination method
2. Method of constrained variation
3. Method of Lagrange multipliers

Variable Elimination Method

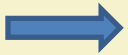
An equality constrained optimization problem can, in principle, be solved by converting it to an unconstrained problem by explicitly eliminating m independent variables using the m equality constraints.

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{x}) \\ \text{subject to:} \quad & h_i(\mathbf{x}) = 0 \; \forall i = 1, 2, \ldots m \\ & \mathbf{x} \in \mathbb{R}^n \end{aligned}$$

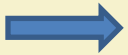
Example:

$$\min_{x_1, x_2} f(\mathbf{x}) = 4x_1^2 + 5x_2^2 + 10$$

$$\text{s.t. } 2x_1 + 3x_2 = 6$$



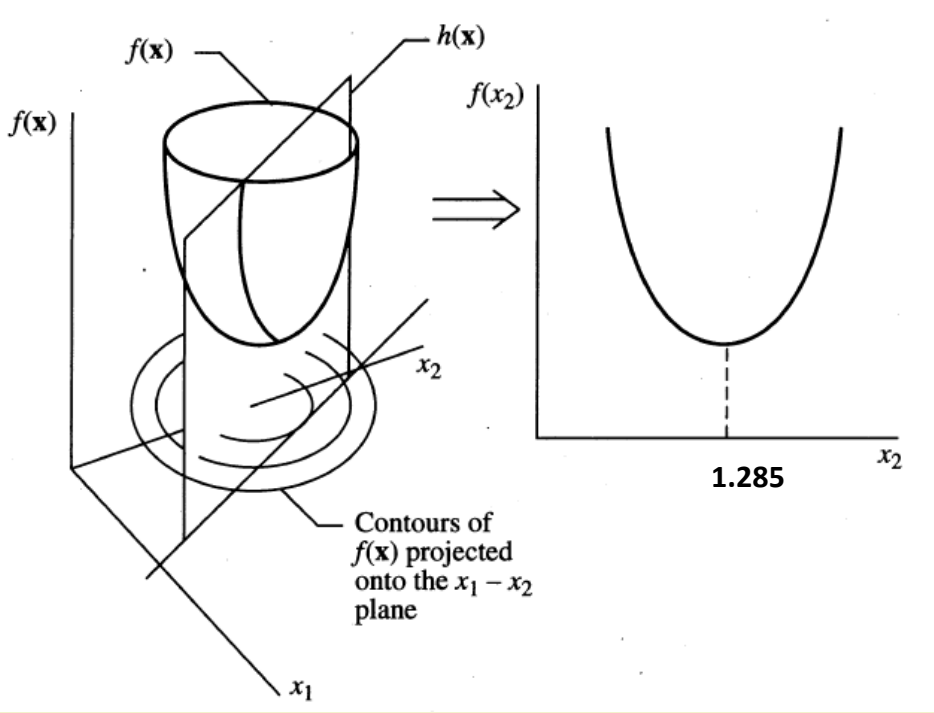
Use: $x_1 = \dfrac{6 - 3x_2}{2}$



$$\min_{x_2} f(x_2) = (6 - 3x_2)^2 + 5x_2^2 + 10$$

Now the optimality criteria for unconstrained problems can be used to find the optimal solution. You can use both necessary and sufficient conditions.

Geometric Interpretation of Elimination Method



$$f(\mathbf{x}) = 4x_1^2 + 5x_2^2 + 10$$

$$h(\mathbf{x}) = 2x_1 + 3x_2 = 6$$

The objective function is the surface of a paraboloid in three-dimensional space.

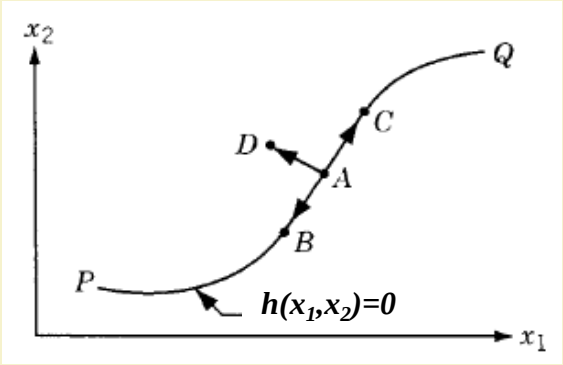
The projection of the intersection of the paraboloid and the plane representing the constraint onto the $f(x_2) = x_2$ plane is a parabola. We then find the minimum of the resulting parabola.

Method of Constrained Variation

Let us consider a two-variable function with a single equality constraint:

Minimize $f(x_1,x_2)$

subject to $h(x_1,x_2) = 0$



If $f(x_1,x_2)$ has a minimum at $x^* = (x_1^*,x_2^*)$, a necessary condition is that the total derivative of $f(x_1,x_2)$ must be zero at (x_1^*,x_2^*):

$$df = \frac{\partial f}{\partial x_1} dx_1 + \frac{\partial f}{\partial x_2} dx_2 = 0$$

Since $h(x_1^*,x_2^*) = 0$ at the minimum point, any variations dx_1 and dx_2 about the point (x_1^*, x_2^*) are *admissible variations* if the point lies on the constraint. That is:

$$h(x_1^* + dx_1 , x_2^* + dx_2) = 0$$

Method of Constrained Variation (Cont'd)

The Taylor series expansion of the function $h(x_1^* + dx_1, x_2^* + dx_2) = 0$ about (x_1^*, x_2^*) gives:

$$h(x_1^* + dx_1, x_2^* + dx_2) = h(x_1^*, x_2^*) + \frac{\partial h}{\partial x_1}(x_1^*, x_2^*)\, dx_1 + \frac{\partial h}{\partial x_2}(x_1^*, x_2^*)\, dx_2 = 0$$

where dx_1 and dx_2 are small

Since $h(x_1^*, x_2^*) = 0$,

$$dh = \frac{\partial h}{\partial x_1} dx_1 + \frac{\partial h}{\partial x_2} dx_2 = 0 \quad \text{at } (x_1^*, x_2^*)$$

This is the condition that must be satisfied for all *admissible variations*.

If we assume: $\partial h / \partial x_2 \neq 0$ we can write

$$dx_2 = -\left.\frac{\partial h / \partial x_1}{\partial h / \partial x_2}\right|_{(x_1^*, x_2^*)} dx_1$$

The equation indicates that once variation along x_1 (dx_1) is chosen arbitrarily, the variation along x_2 (dx_2) is decided automatically to satisfy the condition for the *admissible variation*.

Method of Constrained Variation (Cont'd)

Now combining $df = \frac{\partial f}{\partial x_1} dx_1 + \frac{\partial f}{\partial x_2} dx_2 = 0$ and $dx_2 = -\frac{\partial h / \partial x_1}{\partial h / \partial x_2}(x_1^*, x_2^*) dx_1$

we get: $$df = \left(\frac{\partial f}{\partial x_1} - \frac{\partial h / \partial x_1}{\partial h / \partial x_2} \frac{\partial f}{\partial x_2} \right)\Bigg|_{(x_1^*, x_2^*)} dx_1 = 0$$

The above equation represents constrained variation of f. This must be satisfied for all values of dx_1. Since dx_1 is arbitrary (may be positive/negative), we must have

$$\left(\frac{\partial f}{\partial x_1} \frac{\partial h}{\partial x_2} - \frac{\partial f}{\partial x_2} \frac{\partial h}{\partial x_1} \right)\Bigg|_{(x_1^*, x_2^*)} = 0$$

This is the necessary condition for (x_1^*, x_2^*) to be an extreme point (maximum or minimum).

Method of Constrained Variation: Example

Consider again:

$$\min_{x_1, x_2} f(\mathbf{x}) = 4x_1^2 + 5x_2^2 + 10$$

$$\text{s.t. } h(\mathbf{x}) = 2x_1 + 3x_2 = 6$$

The necessary condition for (x_1^*, x_2^*) to be an extreme point (maximum or minimum) is:

$$\left(\frac{\partial f}{\partial x_1}\frac{\partial h}{\partial x_2} - \frac{\partial f}{\partial x_2}\frac{\partial h}{\partial x_1} \right)\Bigg|_{(x_1^*, x_2^*)} = 0$$

$$\frac{\partial f}{dx_1} = 8x_1, \quad \frac{\partial f}{\partial x_2} = 10x_2$$

$$\frac{\partial h}{\partial x_1} = 2, \quad \frac{\partial h}{\partial x_2} = 3$$

$$3(8x_1) - 2(10x_2) = 0$$

$$\Rightarrow 24x_1 - 20x_2 = 0$$

$$\Rightarrow x_1 = \frac{20x_2}{24} = \frac{5x_2}{6}$$

From, $h(\mathbf{x}) = 2x_1 + 3x_2 = 6$

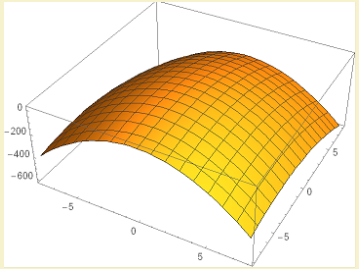
$$\frac{5x_2}{3} + 3x_2 = 6$$

$$\Rightarrow x_2^* = \frac{18}{14} = 1.285$$

Now, $x_1^* = \frac{5x_2^*}{6} = \frac{5(1.285)}{6} = 1.071$

NOTE: The same solution was also obtained when we used Variable Elimination Method.

Optimization in Chemical Engineering



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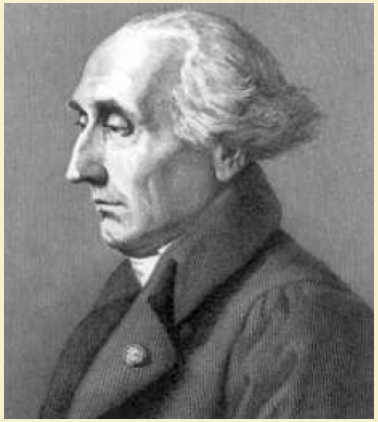
- Lagrange multipliers

Method of Lagrange Multipliers

The method of Lagrange multipliers gives a set of necessary conditions for candidate optimal solutions of equality-constrained optimization problems.

In this method, an equality-constrained problem is converted to an equivalent unconstrained problem with help of certain unspecified parameters known as Lagrange Multipliers.

Each equality constraint is associated with a Lagrange multiplier. Their values depend on the form of the cost and constraint functions. If the functional form of a constraint changes, the value of its Lagrange multiplier also changes.



Joseph-Louis Lagrange
(1736-1813)

Method of Lagrange Multipliers: A Single Equality Constraint

Consider: $\min_{x_1,x_2} f(x_1,x_2)$

$$\text{s.t. } h(x_1,x_2)=0$$

The method of Lagrange multipliers converts this constrained problem to the following unconstrained problem: $L(x_1,x_2,\lambda)=f(x_1,x_2)+\lambda h(x_1,x_2)$

Here the unconstrained function $L(x_1,x_2,\lambda)$ is known as the Lagrangian function, and λ is an unspecified parameter known as Lagrange multiplier. There is no sign restriction on Lagrange multipliers.

If for a given value of λ^* the unconstrained minimum of L occurs at $\mathbf{x}^*$ and $\mathbf{x}^*$ also satisfies $h(\mathbf{x}^*)=0$, then $\mathbf{x}^*$ minimize the original unconstrained problem: Min $L(\mathbf{x}^*,\lambda^*)$ = Min $f(\mathbf{x})$

Method of Lagrange Multipliers: A Single Equality Constraint (Cont'd)

The Lagrangian function: $L(x_1, x_2, \lambda) = f(x_1, x_2) + \lambda h(x_1, x_2)$

Considering L as an unconstrained function of x_1, x_2 and λ, the necessary conditions for its extremum can be written as:

$$\frac{\partial L}{\partial x_1}(x_1, x_2, \lambda) = \frac{\partial f}{\partial x_1}(x_1, x_2) + \lambda \frac{\partial h}{\partial x_1}(x_1, x_2) = 0$$

$$\frac{\partial L}{\partial x_2}(x_1, x_2, \lambda) = \frac{\partial f}{\partial x_2}(x_1, x_2) + \lambda \frac{\partial h}{\partial x_2}(x_1, x_2) = 0$$

$$\frac{\partial L}{\partial \lambda}(x_1, x_2, \lambda) = h(x_1, x_2) = 0$$

Solve simultaneously

Let the solution be: $\left(x_1^*, x_2^*, \lambda^*\right)$

This is a candidate solution.

If Hessian matrix of L at the solution is positive definite, the solution is a local minimum.

If Hessian matrix of L at the solution is negative definite, the solution is a local maximum.

Method of Lagrange Multipliers: General Problem

Consider: Minimize $f(\mathbf{x})$ $\mathbf{x}$ = n-vector
subject to $h_j(\mathbf{x}) = 0$, $j = 1, 2, \ldots, m$

L is now a function of $(n + m)$ unknowns:

$$L(x_1, x_2, ..., x_n, \lambda_1, \lambda_2, ..., \lambda_m) = f(\mathbf{x}) + \lambda_1 h_1(\mathbf{x}) + \lambda_2 h_2(\mathbf{x}) + ... + \lambda_m h_m(\mathbf{x}) = f(\mathbf{x}) + \sum_{j=1}^{m} \lambda_j h_j$$

The necessary conditions are given as:

$$\frac{\partial L}{\partial x_i} = \frac{\partial f}{\partial x_i}(\mathbf{x}) + \sum_{j=1}^{m} \lambda_j \frac{\partial h_j}{\partial x_i}(\mathbf{x}) = 0, \quad i = 1, 2, ..., n \quad j = 1, 2, ..., m$$

$$\frac{\partial L}{\partial \lambda_j} = h_j(\mathbf{x}) = 0, \quad j = 1, 2, ..., m$$

NOTE: There may be multiple solutions. Also, numerical methods may be required for solution.

Solution to the set of equations:

$$\mathbf{x} = \begin{bmatrix} x_1^* \\ x_2^* \\ \vdots \\ x_n^* \end{bmatrix} \qquad \lambda^* = \begin{bmatrix} \lambda_1^* \\ \lambda_2^* \\ \vdots \\ \lambda_m^* \end{bmatrix}$$

Method of Lagrange Multipliers: General Problem: Vector Notation

$$\min_{\mathbf{x}} f(\mathbf{x}), \qquad \mathbf{x} \in \Re^{\mathbf{n}}$$

subject to: $\mathbf{h}(\mathbf{x}) = \mathbf{0}$, m constraints $(m \leq n)$

Define the Lagrange function: $L(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \boldsymbol{\lambda}^T \mathbf{h}(\mathbf{x}), \quad \lambda \in \Re^m$

The stationary points are obtained from:

$$\nabla_{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\lambda}) = \nabla_{\mathbf{x}} f(\mathbf{x}) + \boldsymbol{\lambda}^T \nabla \mathbf{h}(\mathbf{x}) = \mathbf{0}$$

$$\nabla_{\boldsymbol{\lambda}} L(\mathbf{x}, \boldsymbol{\lambda}) = \mathbf{h}(\mathbf{x}) = \mathbf{0}$$

Lagrange Multipliers: Geometric Meaning

$$\min_{x_1, x_2} f(x_1, x_2) = (x_1 - 1.5)^2 + (x_2 - 1.5)^2$$

$$\text{subject to}: h(x_1, x_2) = x_1 + x_2 - 2 = 0$$

Solution: $x_1^* = 1,\ x_2^* = 1,\ \lambda^* = 1$

At optimal point, the gradient of the objective function and the gradient of the constraint function are along the same line and proportional to each other. The Lagrange multiplier is the proportionality constant.

Compare point C and D: C is optimal, not D

$$\frac{\partial f}{\partial x_1} = 2(x_1 - 1.5),\ \frac{\partial f}{\partial x_2} = 2(x_2 - 1.5)$$

$$\frac{\partial h}{\partial x_1} = 1,\ \frac{\partial h}{\partial x_2} = 1$$

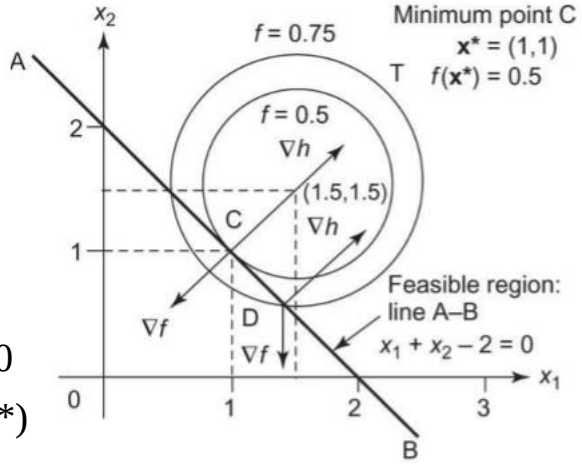
At optimal point C (1,1):

$$\nabla f(\mathbf{x}^*) = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

$$\nabla h(\mathbf{x}^*) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\nabla f(\mathbf{x}^*) + \lambda \nabla h(\mathbf{x}^*) = 0$$

$$\Rightarrow \nabla f(\mathbf{x}^*) = -\lambda \nabla h(\mathbf{x}^*)$$



Sign of Lagrange Multipliers for Equality Constraints

Equality constraints can be multiplied by -1 without affecting the minimum point:

$$\min_{x_1, x_2} f(x_1, x_2) = (x_1 - 1.5)^2 + (x_2 - 1.5)^2$$

$$\text{subject to}: h(x_1, x_2) = -x_1 - x_2 + 2 = 0$$

The optimum solution is same: $x_1^* = 1,\ x_2^* = 1$

But now, $\nabla h(x^*) = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$

Thus the sign of Lagrange multiplier is reversed: $\lambda^* = -1$

λ is free in sign, sign depends on form of *h*

$$\frac{\partial f}{\partial x_1} = 2(x_1 - 1.5),\ \frac{\partial f}{\partial x_2} = 2(x_2 - 1.5)$$

Note the change

$$\frac{\partial h}{\partial x_1} = -1,\ \frac{\partial h}{\partial x_2} = -1$$

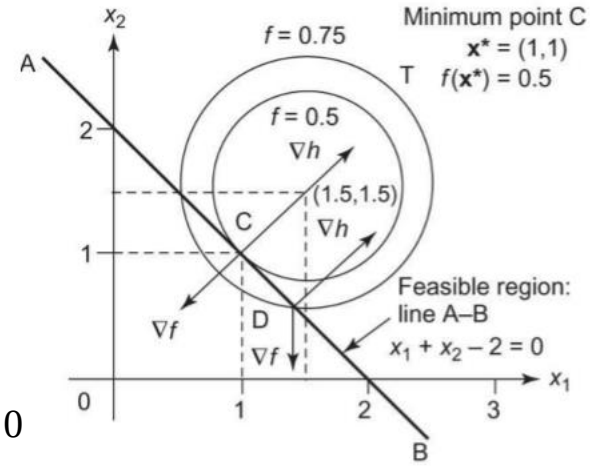
At optimal point C (1,1):

$$\nabla f(\mathbf{x}^*) = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

$$\nabla h(\mathbf{x}^*) = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

$$\nabla f(\mathbf{x}^*) + \lambda \nabla h(\mathbf{x}^*) = 0$$

$$\Rightarrow \nabla f(\mathbf{x}^*) = -\lambda \nabla h(\mathbf{x}^*)$$



Economic Interpretation of Lagrange Multipliers

The Lagrange multiplier, λ, represents the effect of a small change in the constraint on the optimal value of the objective function.

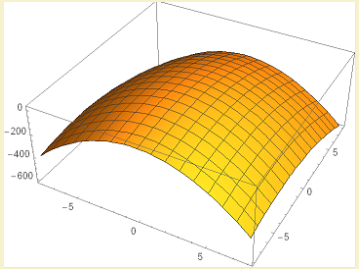
$$\min_{x_1,\ldots,x_n} f(x_1,\ldots,x_n)$$
$$\text{s.t. } h_j(x_1,\ldots,x_n) = 0, \quad j = 1,\ldots,m$$

$$\min_{\mathbf{x}} f(\mathbf{x})$$
$$\text{s.t. } h_j(\mathbf{x}) = b_j, \quad j = 1,\ldots,m$$

Note the change in the RHS of the constraints. Then it can be shown that: $\dfrac{\partial f^*}{\partial b_j} = \lambda_j^*$

Rate of change of optimal value of f with respect to b is given by the optimal value of the Lagrange multiplier. The change in the optimal value of the optimal function per unit increase in the RHS constant of a constraint is given by the Lagrange multiplier. This is known as the shadow price.

Optimization in Chemical Engineering



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- General Nonlinear Programming Problems
- Inequality constraints

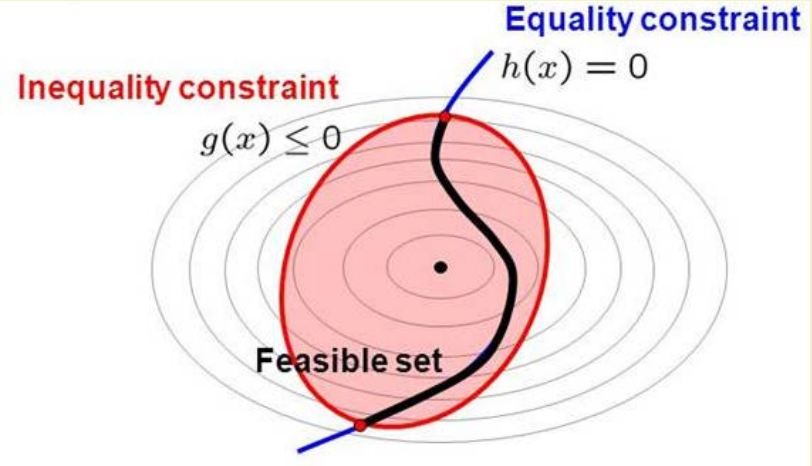
General Nonlinear Programming Problems

The general form:

$$\underset{\mathbf{x}}{\text{Minimize}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{Subject to} \quad g_j(\mathbf{x}) \le 0 \quad \text{for} \quad j = 1, 2, ..., p$$

$$h_k(\mathbf{x}) = 0 \quad \text{for} \quad k = 1, 2, ..., m$$



Active and Inactive Constraints

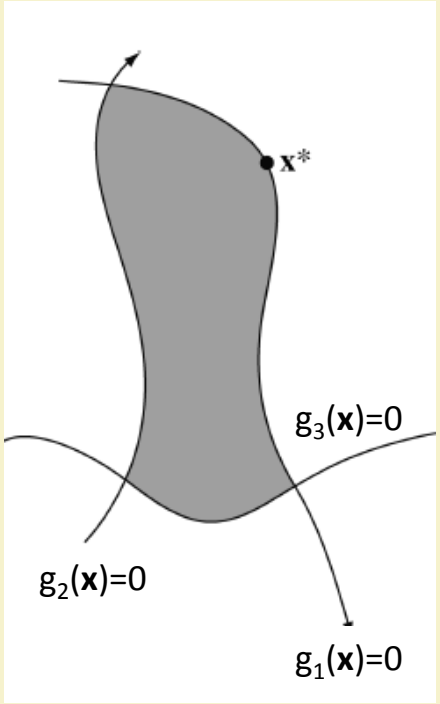
An inequality constraint $g_i(\mathbf{x}^*) \leq 0$ is said to be active (binding) at a feasible point **x*** if the constraint is satisfied as $g_i(\mathbf{x}^*) < 0$.

The inequality constraint is inactive (nonbinding) at **x*** if $g_i(\mathbf{x}^*) = 0$.

An equality constraint $h_i(\mathbf{x}) = 0$ is always as active at any feasible point.

The constraints active at a feasible point **x*** restrict the domain of feasibility in neighborhoods of **x***, while the inactive constraints have no influence in neighborhoods of **x***.

At x*, g_1 is active constraint, g_2 and g_3 are inactive constraints.



Regular Points

Consider: $\min_{\mathbf{x}} f(\mathbf{x})$

$\text{s.t. } \boldsymbol{h}(\mathbf{x}) = 0$

$\min_{\mathbf{x}} f(\mathbf{x})$

$\text{s.t. } \mathbf{g}(\mathbf{x}) \leq 0$

$\boldsymbol{h}(\mathbf{x}) = 0$

A point $\mathbf{x}^*$ satisfying the constraints $\mathbf{h}(\mathbf{x}^*) = 0$ is said to be a regular point of the feasible set if $f(\mathbf{x}^*)$ is differentiable and gradient vectors of all constraints at the point $\mathbf{x}^*$ are linearly independent.

Liner independence means that no two gradients are parallel to each other, and no gradient can be expressed as linear combination of others.

When inequality constraints are also present, then for a point to be regular, gradients of all of the active constraints including inequalities must also be linearly independent.

Theorem: Lagrange Multiplier

Consider: $\min_{\mathbf{x}} f(\mathbf{x})$ s.t. $\boldsymbol{h}(\mathbf{x}) = 0$ $\Leftrightarrow$ $\underset{\mathbf{x}}{\text{Minimize}} \quad f(\mathbf{x})$ $\quad \mathbf{x} = [x_1, x_2, ..., x_n]^T$ Subject to $h_k(\mathbf{x}) = 0$ for $k = 1, 2, ..., m$

Assume **x*** is a regular point of **h**(**x**) = 0 and let **x*** be a local extremum of *f* subject to **h**(**x**) = 0. Then there exists m unique Lagrange multipliers $\lambda \in \Re^m$ such that

$$\nabla L(\mathbf{x}^*, \lambda) = \nabla f(\mathbf{x}^*) + \boldsymbol{\lambda}^T \nabla \mathbf{h}(\mathbf{x}^*) = 0 \quad \Leftrightarrow$$

$$\frac{\partial L(\mathbf{x}, \lambda)}{\partial x_i} = \frac{\partial f(\mathbf{x})}{\partial x_i} + \sum_{j=1}^{m} \lambda_j \frac{\partial h_j(\mathbf{x})}{\partial x_i} = 0 \qquad i = 1, 2, ..., n$$

$$\frac{\partial L(\mathbf{x}, \lambda)}{\partial \lambda_j} = h_j(\mathbf{x}), \quad j = 1, ..., m$$

Lagrange Multipliers: Inequality Constraints

$$\underset{\mathbf{x}}{\text{Minimize}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{Subject to } g_j(\mathbf{x}) \le 0 \quad \text{for } j = 1, 2, ..., p$$

The inequality is of ≤ type. The value of g can be zero or negative.

We can convert such a constraint to an equality constraint by adding a "slack variable". This slack variable must be ≥ 0.

$$g_j(\mathbf{x}) \le 0$$

$$\Rightarrow g_j(\mathbf{x}) + \sigma_j^2 = 0$$

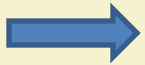
$$\text{Note: } \sigma_j^2 \ge 0$$

σ^2	g	Conclusion
$\sigma^2 = 0$	g = 0	Constraint satisfied, active (Tight constraint, no "slack")
$\sigma^2 > 0$	g < 0	Constraint satisfied, inactive

Lagrange Multipliers: Inequality Constraints

$$\underset{\mathbf{x}}{\text{Minimize}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{Subject to } g_j(\mathbf{x}) \le 0 \quad \text{for } j = 1, 2, ..., p$$



$$\underset{\mathbf{x}}{\text{Minimize}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{Subject to } g_j(\mathbf{x}) + \sigma_j^2 = 0 \quad \text{for } j = 1, 2, ..., p$$

Define the Lagrangian:

$$L(\mathbf{x}, \lambda, \sigma) = f(\mathbf{x}) + \sum_{j=1}^{p} \lambda_j \left(g_j(\mathbf{x}) + \sigma_j^2 \right)$$

If x* is a regular point, then the first-order necessary conditions for x* being an extremum can be obtained by setting the gradient of L to zero.

Lagrange Multipliers: Inequality Constraints

The Lagrangian: $L(\mathbf{x}, \lambda, \sigma) = f(\mathbf{x}) + \sum_{j=1}^{p} \lambda_j \left(g_j(\mathbf{x}) + \sigma_j^2 \right)$

If $\mathbf{x}^* = [x_1^*, x_2^*, \ldots x_n^*]$ is a regular point that is a local minimum of $f(\mathbf{x})$, then the necessary conditions are:

$$\frac{\partial L(\mathbf{x}, \lambda, \sigma)}{\partial x_i} = \frac{\partial f(\mathbf{x})}{\partial x_i} + \sum_{j=1}^{m} \lambda_j \frac{\partial g_j(\mathbf{x})}{\partial x_i} = 0 \qquad i = 1, 2, \ldots, n$$

(gradient condition)

$$\frac{\partial L(\mathbf{x}, \lambda, \sigma)}{\partial \lambda_j} = g_j(\mathbf{x}) + \sigma_j^2 = 0, \quad j = 1, 2, \ldots, p$$

$$\sigma_j^2 \geq 0, \quad j = 1, 2, \ldots, p$$

(non-negativity)

$$\frac{\partial L(\mathbf{x}, \lambda, \sigma)}{\partial \sigma_j} = 2\lambda_j \sigma_j = 0, \quad j = 1, 2, \ldots, p$$

(switching condition)

$$\lambda_j \geq 0 \qquad j = 1, 2, \ldots, p$$ (non-negativity)

Note: Lagrange multipliers for $g \leq 0$ are nonnegative.

If $g_j < 0$, then $\lambda_j = 0$ If $g_j = 0$, then $\lambda_j \geq 0$

Non-negativity of Inequality Constraints

For a minimization problem, if the inequality constraints are of $g \leq 0$ type, then the corresponding Lagrange multiplier are nonnegative ($\lambda \geq 0$).

Let x* be local minimum. Constraint type: $g_j(x) \leq 0$. Consider the first-order perturbations for f and g at the local minimum for feasible nonzero perturbations:

Necessary condition:

$$\frac{\partial f}{\partial x^*} + \lambda \frac{\partial g}{\partial x^*} = 0$$

$\geq 0 \qquad \leq 0$

Hence, $\lambda \geq 0$

$$f(x) - f(x^*) = \frac{df(x^*)}{dx}\Delta x + O_2$$

$$\Rightarrow \frac{df(x^*)}{dx}\Delta x \geq 0$$

$$g(x) - g(x^*) = \frac{dg(x^*)}{dx}\Delta x + O_2$$

$$\Rightarrow \frac{dg(x^*)}{dx}\Delta x \leq 0$$

In case of minimization problems, if the constraints are of the form $g_j(x) \geq 0$, then λ_j have to be non-positive ($\lambda_j \leq 0$).

Non-negativity of Inequality Constraints (Cont'd)

For a minimization problem, if the inequality constraints are of $g \leq 0$ type, then the corresponding Lagrange multiplier are nonnegative ($\lambda \geq 0$).

Also note the following:

Having $\lambda_i \geq 0$ ensures that $L = f(x) + \sum_{i=1}^{p} \lambda_i \left(g_i(x) + \sigma_i^2 \right)$ has a well defined minimum.

If $\lambda_i < 0$, we can always make L smaller due to the presence of $\lambda_i \sigma_i^2$ term.

Inequality Constraints: Necessary Conditions: Alternate Form

$$L(\mathbf{x},\lambda,\sigma) = f(\mathbf{x}) + \sum_{j=1}^{p} \lambda_j \left(g_j(\mathbf{x}) + \sigma_j^2 \right)$$

$$\min_{\mathbf{x}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{s.t. } g_j(\mathbf{x}) \le 0 \quad \text{for } j = 1, 2, ..., p$$

$$\frac{\partial L(\mathbf{x},\lambda,\sigma)}{\partial x_i} = \frac{\partial f(\mathbf{x})}{\partial x_i} + \sum_{j=1}^{m} \lambda_j \frac{\partial g_j(\mathbf{x})}{\partial x_i} = 0 \qquad i = 1, 2, ..., n$$

$$\left.\begin{aligned} &\frac{\partial L(\mathbf{x},\lambda,\sigma)}{\partial \lambda_j} = g_j(\mathbf{x}) + \sigma_j^2 = 0, \quad j = 1, 2, ..., p \\ &\sigma_j^2 \ge 0, \quad j = 1, 2, ..., p \end{aligned}\right\} \Leftrightarrow g_j(\mathbf{x}) \le 0, \quad j = 1, 2, ..., p$$

(feasibility condition)

$$\frac{\partial L(\mathbf{x},\lambda,\sigma)}{\partial \sigma_j} = 2\lambda_j \sigma_j = 0, \quad j = 1, 2, ..., p \qquad \Leftrightarrow \lambda_j g_j = 0, \quad j = 1, 2, ..., p$$

(switching condition)

$$\lambda_j \ge 0 \qquad j = 1, 2, ..., p$$

Inequality Constraints: Necessary Conditions: Alternate Form (Cont'd)

$$\min_{\mathbf{x}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{s.t. } g_j(\mathbf{x}) \le 0 \quad \text{for } j = 1, 2, ..., p$$

The Lagrangian:

$$L(\mathbf{x}, \lambda, \sigma) = f(\mathbf{x}) + \sum_{j=1}^{p} \lambda_j \left(g_j(\mathbf{x}) + \sigma_j^2 \right)$$

Necessary conditions:

$$\frac{\partial L(\mathbf{x}, \lambda, \sigma)}{\partial x_i} = \frac{\partial f(\mathbf{x})}{\partial x_i} + \sum_{j=1}^{m} \lambda_j \frac{\partial g_j(\mathbf{x})}{\partial x_i} = 0 \qquad i = 1, 2, ..., n$$

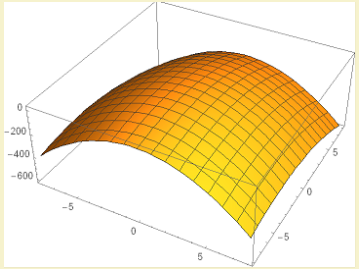
(gradient condition)

$g_j(\mathbf{x}) \le 0, \quad j = 1, 2, ..., p$ (feasibility condition

$\lambda_j g_j = 0, \quad j = 1, 2, ..., p$ (switching condition)

$\lambda_j \ge 0 \qquad j = 1, 2, ..., p$ (non-negativity condition)

Optimization in Chemical Engineering



Thank You

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CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Basic Concepts of Optimization – II

(WEEK – 4: LECTURE – 19)

Dr. Debasis Sarkar

Department of Chemical Engineering

Indian Institute of Technology Kharagpur

Basic Concepts of Optimization – II

Week 4:

- Equality constrained problems: Introduction
- Variable elimination method
- Method of constrained variation
- Lagrange multipliers
- General Nonlinear Programming Problems
- Kuhn Tucker conditions

Today's Topic:

- Kuhn Tucker conditions

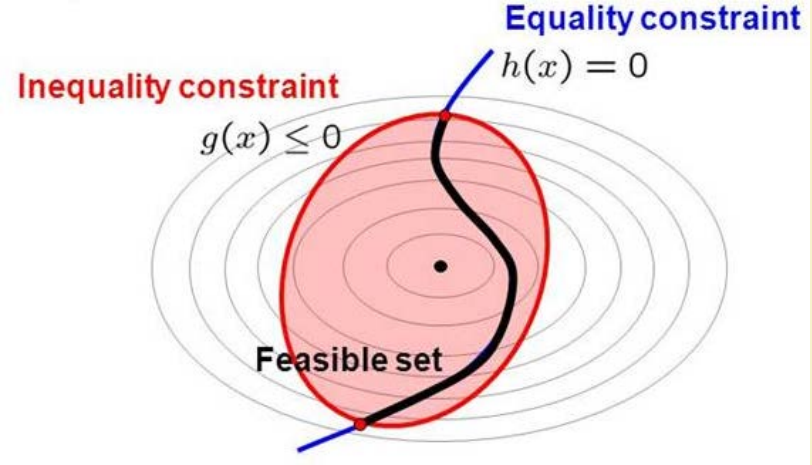
General Nonlinear Programming Problems: Review

The general form:

$$\underset{\mathbf{x}}{\text{Minimize}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{Subject to} \quad g_j(\mathbf{x}) \le 0 \quad \text{for} \quad j = 1, 2, ..., p$$

$$h_k(\mathbf{x}) = 0 \quad \text{for} \quad k = 1, 2, ..., m$$



Equality/Inequality Constraints: Necessary Conditions

Equality constraints

$$\min_{\mathbf{x}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{s.t. } h_j(\mathbf{x}) = 0 \quad \text{for } j = 1, 2, ..., m$$

The Lagrangian: $L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \sum_{j=1}^{m} \lambda_j h_j$

Necessary conditions:

$$\frac{\partial L}{\partial x_i} = \frac{\partial f}{\partial x_i}(\mathbf{x}) + \sum_{j=1}^{m} \lambda_j \frac{\partial h_j}{\partial x_i}(\mathbf{x}) = 0,$$

$$i = 1, 2, ..., n \qquad j = 1, 2, ..., m$$

$$\frac{\partial L}{\partial \lambda_j} = h_j(\mathbf{x}) = 0, \qquad j = 1, 2, ..., m$$

Inequality constraints

$$\min_{\mathbf{x}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{s.t. } g_j(\mathbf{x}) \le 0 \quad \text{for } j = 1, 2, ..., p$$

The Lagrangian: $L(\mathbf{x}, \lambda, \sigma) = f(\mathbf{x}) + \sum_{j=1}^{p} \lambda_j \left(g_j(\mathbf{x}) + \sigma_j^2 \right)$

Necessary conditions:

$$\frac{\partial L(\mathbf{x}, \lambda, \sigma)}{\partial x_i} = \frac{\partial f(\mathbf{x})}{\partial x_i} + \sum_{j=1}^{m} \lambda_j \frac{\partial g_j(\mathbf{x})}{\partial x_i} = 0, \; i = 1, 2, ..., n$$

$$g_j(\mathbf{x}) \le 0, \quad j = 1, 2, ..., p$$

$$\lambda_j g_j = 0, \quad j = 1, 2, ..., p$$

$$\lambda_j \ge 0 \qquad j = 1, 2, ..., p$$

If we sum up these necessary conditions, we get Karush – Kuhn – Tucker (KKT) conditions

Karush – Kuhn – Tucker (KKT) Conditions

$$\underset{\mathbf{x}}{\text{Minimize}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{Subject to } g_j(\mathbf{x}) \le 0 \quad \text{for } j = 1, 2, ..., p$$

$$h_k(\mathbf{x}) = 0 \quad \text{for } k = 1, 2, ..., m$$

The Lagrangian:

$$L(\mathbf{x}, \boldsymbol{u}, \boldsymbol{v}) = f(\mathbf{x}) + \sum_{i=1}^{m} v_i h_i(\mathbf{x}) + \sum_{j=1}^{p} u_j g_j(\mathbf{x})$$

$$\Rightarrow L(\mathbf{x}, \boldsymbol{u}, \boldsymbol{v}) = f(\mathbf{x}) + \boldsymbol{v}^T \mathbf{h}(\mathbf{x}) + \boldsymbol{u}^T \mathbf{g}(\mathbf{x})$$

1. Gradient conditions:

$$\frac{\partial L(\mathbf{x}^*, \boldsymbol{u}^*, \boldsymbol{v}^*)}{\partial x_i} = \frac{\partial f(\mathbf{x}^*)}{\partial x_i} + \sum_{j=1}^{m} v_j^* \frac{\partial h_j(\mathbf{x}^*)}{\partial x_i} + \sum_{j=1}^{p} u_j^* \frac{\partial g_j(\mathbf{x}^*)}{\partial x_i} = 0, \; i = 1, 2, ..., n$$

2. Feasibility check:

$$g_j(\mathbf{x}^*) \le 0, \quad j = 1, 2, ..., p$$

$$h_i(\mathbf{x}^*) = 0, \quad i = 1, 2, ..., m$$

3. Switching conditions: $u_j^* g_j = 0, \quad j = 1, 2, ..., p$

4. Non-negativity of Lagrange multipliers for inequalities: $u_j^* \ge 0, \quad j = 1, 2, ..., p$

5. Regularity check: Gradients of active constraints must be linearly independent.

Karush – Kuhn – Tucker (KKT) Conditions: Theorem

$$\underset{\mathbf{x}}{\text{Minimize}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{Subject to } g_j(\mathbf{x}) \le 0 \quad \text{for } j = 1, 2, ..., p$$

$$h_k(\mathbf{x}) = 0 \quad \text{for } k = 1, 2, ..., m$$

Let **x*** be a regular point and the local minimum for the given NLP problem. Then there exists Lagrange multipliers ***v**** (a m-vector) and ***u**** (a p-vector) such that the Lagrangian function L is stationary with respect to **x**, ***v***, ***u*** at the point **x***. For **x*** to be stationary, the following conditions must be satisfied.

$$L(\mathbf{x}, \boldsymbol{u}, \boldsymbol{v}) = f(\mathbf{x}) + \sum_{i=1}^{m} v_i h_i(\mathbf{x}) + \sum_{j=1}^{p} u_j g_j(\mathbf{x})$$

$$\frac{\partial L(\mathbf{x}^*, \boldsymbol{u}^*, \boldsymbol{v}^*)}{\partial x_i} = \frac{\partial f(\mathbf{x}^*)}{\partial x_i} + \sum_{j=1}^{m} v_j^* \frac{\partial h_j(\mathbf{x}^*)}{\partial x_i} + \sum_{j=1}^{p} u_j^* \frac{\partial g_j(\mathbf{x}^*)}{\partial x_i} = 0, \; i = 1, 2, ..., n$$

$$g_j(\mathbf{x}^*) \le 0, \quad j = 1, 2, ..., p$$

$$h_i(\mathbf{x}^*) = 0, \quad i = 1, 2, ..., m$$

$$u_j^* g_j = 0, \quad j = 1, 2, ..., p$$

$$u_j^* \ge 0, \quad j = 1, 2, ..., p$$

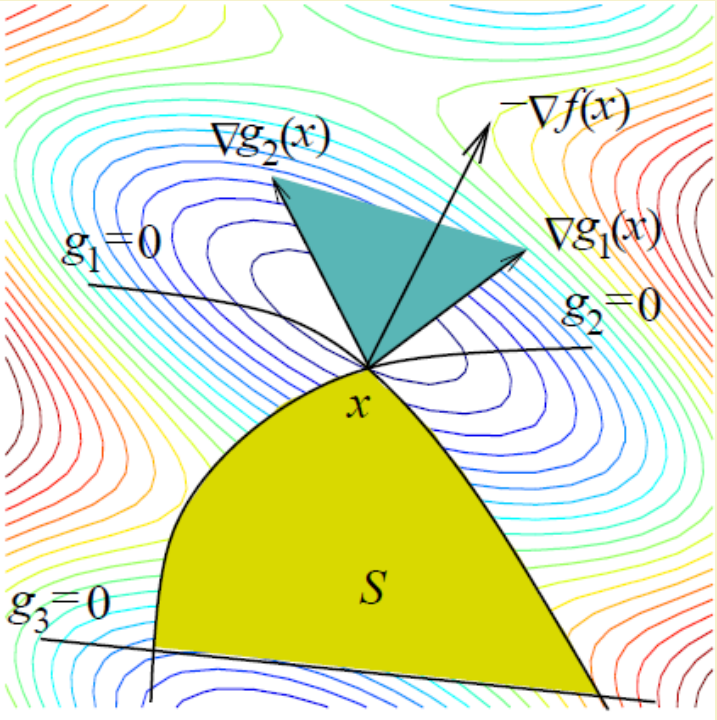
Karush – Kuhn – Tucker (KKT) Conditions: Observations

The KKT conditions are first-order necessary conditions for optimality. The points satisfying KKT conditions are called KKT points.

The KKT conditions are not applicable at the points that are not regular. At irregular points, the use of KKT conditions may yield candidate minimum points – but the Lagrange multipliers associated with the constraints may not be unique.

Any point that does not satisfy the KKT conditions cannot be a local minimum (maximum) unless it is an irregular point. Note that KKT conditions are not applicable for irregular points.

KKT Conditions: Geometric Interpretation



$$-\nabla f(\mathbf{x}^*) = \sum_{j=1}^{m} v_j^* \nabla h(\mathbf{x}^*) + \sum_{j=1}^{p} u_j^* \nabla g(\mathbf{x}^*)$$

At the optimal (here minimum) point x, only the active constraints (g_1 and g_2) are important.

The negative gradient of the objective function can be written as a non-negative sum of the gradient of the active constraints.

KKT: Second Order Necessary Conditions

Let **x*** satisfy the KKT conditions for the general NLP problem. Define the Hessian of the Lagrange function L at **x*** as:

$$\nabla^2 L = \nabla^2 f + \sum_{j=1}^{m} v_j^* \nabla^2 h_j + \sum_{j=1}^{p} u_j^* \nabla^2 g_j$$

Let there be nonzero feasible directions, **d** ≠ 0, satisfying the following linear systems at the point **x***:

$$\nabla h_j^T \boldsymbol{d} = 0, \quad j = 1, 2, \ldots, m$$

$$\nabla g_i^T \boldsymbol{d} = 0, \quad \text{for all active inequalities (for those } j \text{ with } g_j(\mathbf{x}^*) = 0)$$

Then for **x*** to be a local minimum, it must be true that: $Q = \boldsymbol{d}^T \nabla^2 L(\mathbf{x}^*) \boldsymbol{d} \geq 0$

Second-order necessary condition

KKT: Second Order Sufficient Conditions

Let **x*** satisfy the KKT conditions **for** the general NLP problem. Define the Hessian of the Lagrange function L at **x*** as:

$$\nabla^2 L = \nabla^2 f + \sum_{j=1}^{m} v_j^* \nabla^2 h_j + \sum_{j=1}^{p} u_j^* \nabla^2 g_j$$

Let there be nonzero feasible directions, **d** ≠ 0, satisfying the following linear systems at the point **x***:

$$\nabla h_j^T \boldsymbol{d} = 0, \quad j = 1, 2, \ldots, m$$

$$\nabla g_i^T \boldsymbol{d} = 0, \quad \text{for all active inequalities (for those } j \text{ with } g_j(\mathbf{x}^*) = 0)$$

Also let $\nabla g_i^T \boldsymbol{d} \le 0$ for those active inequalities with $u_j^* = 0$.

Then **x*** is a local minimum if : $Q = \boldsymbol{d}^T \nabla^2 L(\mathbf{x}^*) \boldsymbol{d} > 0$ **Second-order sufficient condition**

Karush – Kuhn – Tucker (KKT) Conditions and Convexity

If x* is a local minimum for a convex function *f*(x) that is defined on a convex feasible set S, then it is also a global minimum.

If both the objective function and the feasible region are convex, then the NLP problem is a convex problem.

For a convex problem, we are assured that a global minimum exists and that any point **x*** that satisfies the first-order KKT conditions will be a global minimum.

Karush – Kuhn – Tucker (KKT) Conditions: Example - 1

$$\underset{x_1,x_2}{\text{Min}}\ f(x_1,x_2) = x_1^2 - x_2$$

s.t. $g_1 = x_1 - 1 \geq 0$

$g_2 = 30 - x_1^2 - x_2^2 \geq 0$

$h_1 = x_1 + x_2 - 6 = 0$

$$\underset{x_1,x_2}{\text{Min}}\ f(x_1,x_2) = x_1^2 - x_2$$

s.t. $g_1 = 1 - x_1 \leq 0$

$g_2 = x_1^2 + x_2^2 - 30 \leq 0$

$h_1 = x_1 + x_2 - 6 = 0$

The Lagrangian: $L = \left(x_1^2 - x_2\right) + u_1(1 - x_1) + u_2(x_1^2 + x_2^2 - 30) + v(x_1 + x_2 - 6)$

$$2x_1 - u_1 + 2x_1u_2 + v_1 = 0$$

$$-1 + 2x_2u_2 + v_1 = 0$$

$$1 - x_1 \leq 0$$

$$x_1^2 + x_2^2 - 30 \leq 0$$

$$x_1 + x_2 - 6 = 0$$

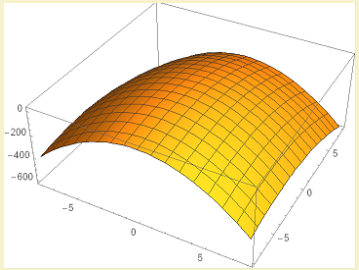
$$u_1\left(1 - x_1\right) = 0$$

$$u_2\left(x_1^2 + x_2^2 - 30\right) = 0$$

$$u_1, u_2 \geq 0$$

v = free in sign

Optimization in Chemical Engineering



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NPTEL ONLINE CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Basic Concepts of Optimization – II

(WEEK – 4: LECTURE – 20)

Dr. Debasis Sarkar

Department of Chemical Engineering

Indian Institute of Technology Kharagpur

Basic Concepts of Optimization – II

Week 4:

- ✓ Equality constrained problems: Introduction
- ✓ Variable elimination method
- ✓ Method of constrained variation
- ✓ Lagrange multipliers
- ✓ General Nonlinear Programming Problems
- ✓ Kuhn Tucker conditions

Today's Topic:

- Kuhn Tucker conditions: Examples

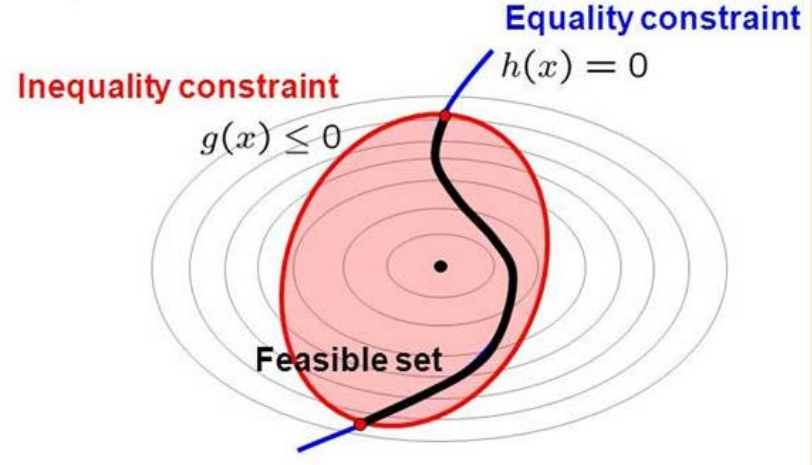
General Nonlinear Programming Problems: Review

The general form:

$$\underset{\mathbf{x}}{\text{Minimize}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{Subject to} \quad g_j(\mathbf{x}) \le 0 \quad \text{for} \quad j = 1, 2, ..., p$$

$$h_k(\mathbf{x}) = 0 \quad \text{for} \quad k = 1, 2, ..., m$$



Karush – Kuhn – Tucker (KKT) Conditions

$$\underset{\mathbf{x}}{\text{Minimize}} \quad f(\mathbf{x}) \qquad \mathbf{x} = [x_1, x_2, ..., x_n]^T$$

$$\text{Subject to } g_j(\mathbf{x}) \le 0 \quad \text{for } j = 1, 2, ..., p$$

$$h_k(\mathbf{x}) = 0 \quad \text{for } k = 1, 2, ..., m$$

The Lagrangian:

$$L(\mathbf{x}, \boldsymbol{u}, \boldsymbol{v}) = f(\mathbf{x}) + \sum_{i=1}^{m} v_i h_i(\mathbf{x}) + \sum_{j=1}^{p} u_j g_j(\mathbf{x})$$

$$\Rightarrow L(\mathbf{x}, \boldsymbol{u}, \boldsymbol{v}) = f(\mathbf{x}) + \boldsymbol{v}^T \mathbf{h}(\mathbf{x}) + \boldsymbol{u}^T \mathbf{g}(\mathbf{x})$$

1. Gradient conditions:

$$\frac{\partial L(\mathbf{x}^*, \boldsymbol{u}^*, \boldsymbol{v}^*)}{\partial x_i} = \frac{\partial f(\mathbf{x}^*)}{\partial x_i} + \sum_{j=1}^{m} v_j^* \frac{\partial h_j(\mathbf{x}^*)}{\partial x_i} + \sum_{j=1}^{p} u_j^* \frac{\partial g_j(\mathbf{x}^*)}{\partial x_i} = 0, \; i = 1, 2, ..., n$$

2. Feasibility check:

$$g_j(\mathbf{x}^*) \le 0, \quad j = 1, 2, ..., p$$

$$h_i(\mathbf{x}^*) = 0, \quad i = 1, 2, ..., m$$

3. Switching conditions: $u_j^* g_j = 0, \quad j = 1, 2, ..., p$

4. Non-negativity of Lagrange multipliers for inequalities: $u_j^* \ge 0, \quad j = 1, 2, ..., p$

5. Regularity check: Gradients of active constraints must be linearly independent.

Inequality Constraints: Example - 1

$$\underset{x_1, x_2}{\text{Minimize}} \quad f(x_1, x_2) = (x_1 - 1.5)^2 + (x_2 - 1.5)^2$$

Subject to $g(x, y) = x_1 + x_2 - 2 \leq 0$

Define Lagrangian:

$$L(x_1, x_2, \lambda, \sigma) = f(x_1, x_2) + \lambda\left(g(x_1, x_2) + \sigma^2\right)$$

$$\Rightarrow L = (x_1 - 1.5)^2 + (x_2 - 1.5)^2 + \lambda(x_1 + x_2 - 2 + \sigma^2)$$

Necessary conditions:

$$\frac{\partial L}{\partial x_1} = 2(x_1 - 1.5) + \lambda = 0$$

$$\frac{\partial L}{\partial x_2} = 2(x_2 - 1.5) + \lambda = 0$$

$$\frac{\partial L}{\partial \lambda} = x_1 + x_2 - 2 + \sigma^2 = 0$$

$$\frac{\partial L}{\partial \sigma} = 2\lambda\sigma = 0$$

$$\lambda \geq 0; \quad \sigma^2 \geq 0$$

4 equations, 4 unknowns: x_1, x_2, λ, σ

Nonlinear equations – multiple solutions possible.

Look at the switching condition: $2\lambda\sigma = 0$. Either $\lambda = 0$, or $\sigma = 0$

Case - A

First set $\sigma = 0$. That is inequality is active: $g = 0$

Solution: $x^*_1 = 1$, $x^*_2 = 1$, $\lambda^* = 1 > 0$, $\sigma^* = 0$

This is a stationary point of L – so candidate minimum point.

Inequality Constraints: Example - 1 (Cont'd)

Necessary conditions:

$$\frac{\partial L}{\partial x_1} = 2(x_1 - 1.5) + \lambda = 0$$

$$\frac{\partial L}{\partial x_2} = 2(x_2 - 1.5) + \lambda = 0$$

$$\frac{\partial L}{\partial \lambda} = x_1 + x_2 - 2 + \sigma^2 = 0$$

$$\frac{\partial L}{\partial \sigma} = 2\lambda\sigma = 0$$

$$\lambda \geq 0; \quad \sigma^2 \geq 0$$

Look at the switching condition: $2\lambda\sigma = 0$. Either $\lambda = 0$, or $\sigma = 0$

Case - B

Now set $\lambda = 0$. That is inequality is inactive: $g < 0$

Solution: $x^*_1 = 1.5$, $x^*_2 = 1.5$, $\lambda^* = 0$, $\sigma^2 = -1 \not\geq 0$

This is not a valid solution as it violates the inequality constraint at point x^* because $g = -\sigma^2 = 1 > 0$

Inequality Constraints: Example: - 1: Geometry

$$\underset{x_1,x_2}{\text{Minimize}} \quad f(x_1,x_2)=(x_1-1.5)^2+(x_2-1.5)^2$$

$$\text{Subject to } g(x,y)=x_1+x_2-2\le 0$$

The feasible region for this inequality constrained problem is the line A-B and the region below it.

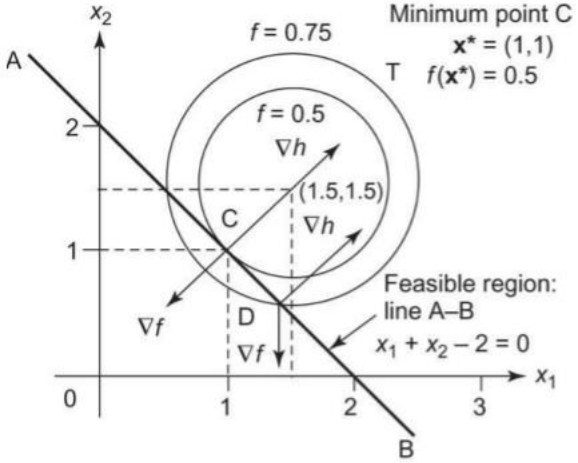
Note: at optimal point:

$$\nabla f=\begin{bmatrix}2(x_1-1.5)\\2(x_1-1.5)\end{bmatrix}=\begin{bmatrix}-1\\-1\end{bmatrix},\quad \nabla g=\begin{bmatrix}1\\1\end{bmatrix}$$

$$\underset{x_1,x_2}{\text{Min}} \ (x_1-1.5)^2+(x_2-1.5)^2$$

$$\text{s.t. } x_1+x_2-2=0$$

Optimal point: C



Inequality Constraints: KKT Conditions: Example - 2

Minimize $f = x_1^2 + 2x_2^2 + 3x_3^2$

subject to $g_1 = x_1 - x_2 - 2x_3 \le 12$

$g_2 = x_1 + 2x_2 - 3x_3 \le 8$

Minimize $f = x_1^2 + 2x_2^2 + 3x_3^2$

subject to $g_1 = x_1 - x_2 - 2x_3 - 12 \le 0$

$g_2 = x_1 + 2x_2 - 3x_3 - 8 \le 0$

The Lagrange function:

$$L = \left(x_1^2 + 2x_2^2 + 3x_3^2\right) + u_1\left(x_1 - x_2 - 2x_3 - 12\right) + u_2\left(x_1 + 2x_2 - 3x_3 - 8\right)$$

Inequality Constraints: KKT Conditions: Example - 2

$$L = \left(x_1^2 + 2x_2^2 + 3x_3^2\right) + u_1\left(x_1 - x_2 - 2x_3 - 12\right) + u_2\left(x_1 + 2x_2 - 3x_3 - 8\right)$$

$$\frac{\partial f}{\partial x_i} + u_1\frac{\partial g_1}{\partial x_i} + u_2\frac{\partial g_2}{\partial x_i} = 0, \quad i = 1,2,3$$

$$2x_1 + u_1 + u_2 = 0 \quad (1)$$
$$4x_2 - u_1 + 2u_2 = 0 \quad (2)$$
$$6x_3 - 2u_1 - 3u_2 = 0 \quad (3)$$

$$u_j g_j = 0$$

$$u_1(x_1 - x_2 - 2x_3 - 12) = 0 \quad (4)$$
$$u_2(x_1 + 2x_2 - 3x_3 - 8) = 0 \quad (5)$$

$$g_j \le 0$$

$$x_1 - x_2 - 2x_3 - 12 \le 0 \quad (6)$$
$$x_1 + 2x_2 - 3x_3 - 8 \le 0 \quad (7)$$

$$u_j \ge 0$$

$$u_1 \ge 0 \quad (8)$$
$$u_2 \ge 0 \quad (9)$$

Inequality Constraints: KKT Conditions: Example – 2 (Cont'd)

From (4): $\left[u_j g_j = 0\right]$ Either $u_1 = 0$ or $(x_1 - x_2 - 2x_3 - 12) = 0$

Case 1: $u_1 = 0$

From (1), (2) and (3), we get: $x_1 = x_2 = -\frac{u_2}{2},\ x_3 = \frac{u_2}{2}$

Put these in (5) and we get: $u_2^2 + 8u_2 = 0, \Rightarrow u_2 = 0 \text{ or } -8$

From (9) $\left[u_j \geq 0\right]$ we can write: $u_2 = 0$

Therefore, $\mathbf{x}^*$ = [0, 0, 0] This solution set satisfies all the conditions.

Inequality Constraints: KKT Conditions: Example – 2 (Cont'd)

Case 2: $x_1 - x_2 - 2x_3 - 12 = 0$

Using (1), (2) and (3), we have:

$$\frac{-u_1 - u_2}{2} - \frac{u_1 - 2u_2}{4} - \frac{2u_1 + 3u_2}{3} - 12 = 0$$

$$\Rightarrow 17u_1 + 12u_2 = -144$$

Since both $u_1 \geq 0$ and $u_2 \geq 0$, it is not possible that $17u_1 + 12u_2 = -144$

Hence the solution set for this optimization problem is: $\mathbf{x}^* = [\,0, 0, 0\,]$

Inequality Constraints: KKT Conditions: Example – 3

Consider the following problem. Does the point $\bar{x} = (\bar{x}_1, \bar{x}_2) = (7, 6)$ satisfy KKT condition?

$$
\begin{array}{lcll}
\min & 6(x_1 - 10)^2 & +4(x_2 - 12.5)^2 & \\
\text{s.t.} & x_1^2 & +(x_2 - 5)^2 & \leq 50 \\
& x_1^2 & +3x_2^2 & \leq 200 \\
& (x_1 - 6)^2 & +x_2^2 & \leq 37
\end{array}
$$

Check feasibility:

$$g_1(\bar{x}) = 0 \leq 0$$

$$g_2(\bar{x}) = -43 < 0$$

$$g_3(\bar{x}) = 0 \leq 0$$

Note: First and third constraints (g_1, g_3) are active. Second constraint (g_2) is inactive.

Inequality Constraints: KKT Conditions: Example – 3

Compute gradients at $\bar{x} = (\bar{x}_1, \bar{x}_2) = (7, 6)$

$$\nabla f(x) = \begin{pmatrix} -36 \\ -52 \end{pmatrix}$$

$$\nabla g_1(x) = \begin{pmatrix} 14 \\ 2 \end{pmatrix}$$

$$\nabla g_2(x) = \begin{pmatrix} 14 \\ 36 \end{pmatrix}$$

$$\nabla g_3(x) = \begin{pmatrix} 2 \\ 12 \end{pmatrix}$$

Note: First and third constraints (g_1, g_3) are active. Second constraint (g_2) is inactive. Gradients of g_1 and g_3 are linearly independent. So the point is a regular point and KKT will apply.

Also note that Lagrange multiplier for inactive constraint should be zero. For others, it will be non-negative.

Inequality Constraints: KKT Conditions: Example – 3

Check the gradient condition at $\bar{x} = (\bar{x}_1, \bar{x}_2) = (7, 6)$

$$\frac{\partial f}{\partial x_i} + u_1 \frac{\partial g_1}{\partial x_i} + u_2 \frac{\partial g_2}{\partial x_i} + u_3 \frac{\partial g_3}{\partial x_i} = 0,\ i = 1, 2$$

$$\begin{pmatrix} -36 \\ -52 \end{pmatrix} + \begin{pmatrix} 14 \\ 2 \end{pmatrix} u_1 + \begin{pmatrix} 14 \\ 36 \end{pmatrix} u_2 + \begin{pmatrix} 2 \\ 12 \end{pmatrix} u_3 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Note that Lagrange multiplier for inactive constraint should be zero. For others, it will be non-negative.

The solution of the system is: $\bar{u} = (\bar{u}_1, \bar{u}_2, \bar{u}_3) = (2, 0, 4)$

Thus: $\bar{u} \geq 0$ $\bar{u}_2 = 0.$

The point $\bar{x} = (\bar{x}_1, \bar{x}_2) = (7, 6)$ satisfies KKT condition and is a candidate for an optimal solution for the problem.

Inequality Constraints: KKT Conditions: Example – 3

$$\underset{x,y}{\text{Minimize}} \quad f(x,y) = 2y - x^2$$

$$\text{Subject to} \quad g_1 = x^2 + y^2 \le 1$$

$$g_2 = x \ge 0$$

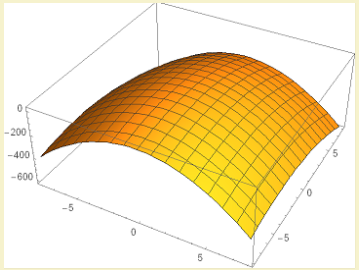
$$g_3 = y \ge 0$$

Formulate the Lagrangian function.

The Lagrange function:

$$L = \left(2y - x^2\right) + u_1\left(x^2 + y^2 - 1\right) + u_2\left(-x\right) + u_3(-y)$$

Optimization in Chemical Engineering



Thank You