



IIT KHARAGPUR



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CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Introduction to Optimization

(WEEK – 1: LECTURE - 1)

Dr. Debasis Sarkar

**Department of Chemical Engineering
Indian Institute of Technology Kharagpur**

Optimization in Chemical Engineering

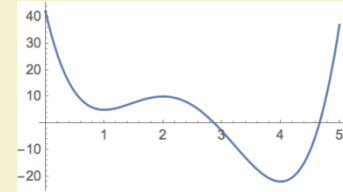
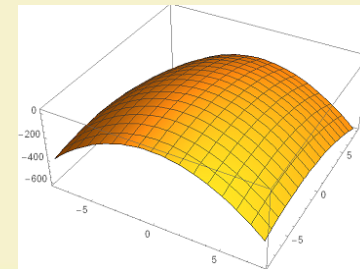
What is optimization?

Finding the best candidate from a set of alternatives without explicitly enumerating and evaluating all possible alternatives.

Origin: Latin word “optimus” which means “best”, “very good”

Optimization is the science of making best possible decision.

By performing optimization, we aim to obtain the best result under given circumstances.



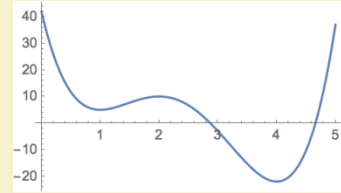
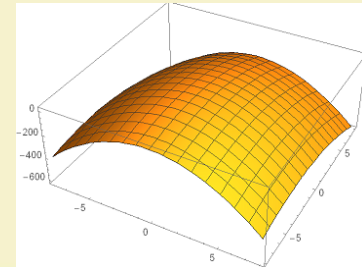
Optimization in Chemical Engineering

Why optimize?

- Improve the process to realize maximum system potential.
- Attain new or improved/more efficient designs; maximize profits; reduce cost of productions.

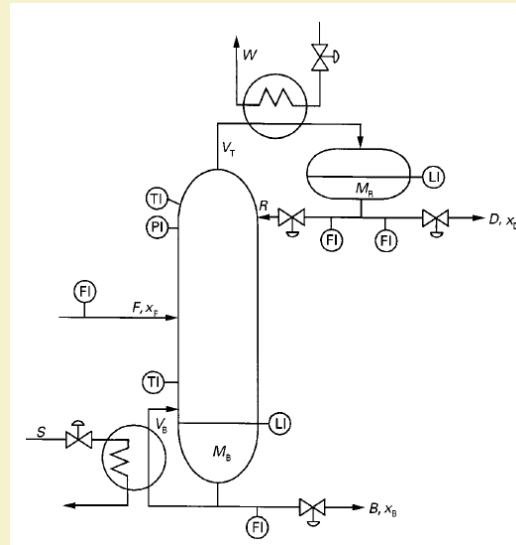
In chemical engineering:

- Utilize resource/energy/utility in the most efficient way
- Reduce waste generation; minimize the environmental impact
- Determine the most desirable operating conditions; Safe operation
- Meet product specification; Maximize profit



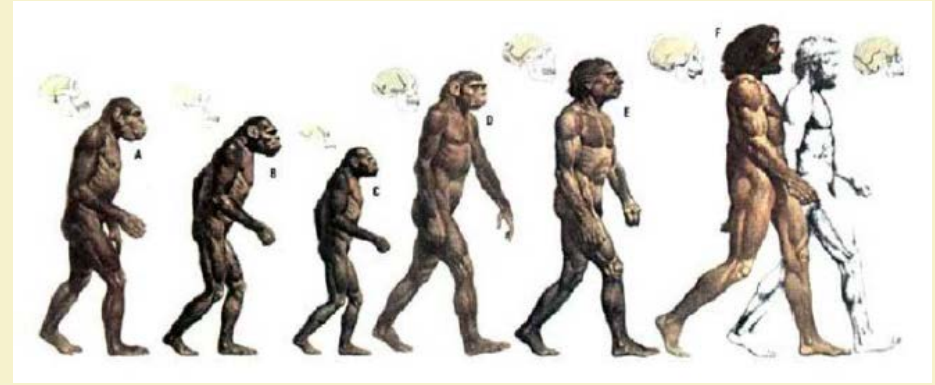
Benefits of Optimization in a Process Plant

In plant operations, benefits of optimization arise from improved plant performance, such as improved yields of valuable products, reduced energy consumption, higher processing rates, reduced maintenance costs, less equipment wear, and longer times between shutdowns.



- Design of a heat exchanger network,
- Real-time optimization of a distillation column,
- Model predictive control,
- Operations planning and scheduling,
- Equipment sizing,
- Scheduling maintenance and equipment replacement,
- Operating equipment, such as reactors and columns.

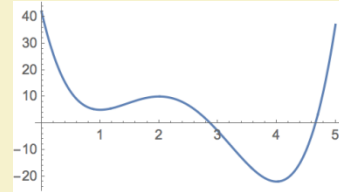
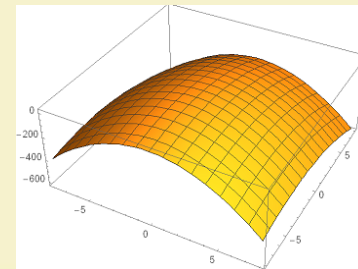
Optimization Examples: Learn from Nature



Optimization in Chemical Engineering

Course Outline

- Week 1 : Introduction to optimization
- Week 2 : Optimization problem formulation
- Week 3 and 4 : Basic concepts of optimization
- Week 5, 6, 7: Unconstrained single and multi-variable optimization
- Week 8 and 9 : Introduction to Linear Programming
- Week 10 : Constrained nonlinear programming
- Week 11 : Applications of optimization
- Week 12 : Software tools for optimization



TEXT/REFERENCE BOOKS

1. Optimization of Chemical Processes – T. F. Edgar, D. M. Himmelblau and L. S. Lasdon, 2nd Edition, McGraw Hill, 2001
2. Engineering Optimization: Methods and Applications - A. Ravindran, K. M. Ragsdell, G. V. Reklaitis, 2nd Edition, Wiley India, 2006
3. Engineering Optimization: Theory and Practice - S. S. Rao, 4th Edition, John Wiley & Sons, Inc, 2009

Scope for Optimization: Wide Areas of Application

1. Production planning (large scale production, best plant site, operating conditions)
2. Transport and logistics (routing of vehicles, allocation of empty wagons, fuel transport)
3. Packing problem (design of cargo space)
4. Telecommunication (design of network, frequency allocation of a mobile network)
5. Traffic planning (traffic signal control)
6. Structural design (mechanical design)
7. Time table, Human resource (staff control)
8. Portfolio optimization (finance)
9. Process control
10. Image analysis (photo conversion, image segmentation)

Plan for Week 1: Introduction to Optimization

Lecture: 1

- ❑ Introduction, Motivation, Text books, etc

Lecture: 2

- ❑ Statement of optimization problems
- ❑ Classification of optimization problems

Lecture: 3

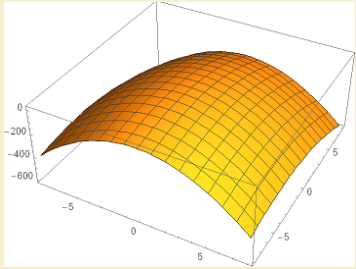
- ❑ Examples of engineering applications

Lecture: 4 and 5

- ❑ Review of linear algebra

Optimization in Chemical Engineering

Thank You





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Introduction to Optimization

(WEEK – 1: LECTURE - 2)

Dr. Debasis Sarkar

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Introduction to Optimization

Week 1:



- ☐ Introduction
- ☐ Statement of optimization problems
- ☐ Classification of optimization problems
- ☐ Examples of engineering applications
- ☐ Review of linear algebra

Today's Topic:

- ☐ Statement of an optimization problem
- ☐ Classification of optimization problems

Statement of an Optimization Problem

All optimization problems are stated in some standard form. You have to identify the essential elements of a given problem and translate them into a prescribed mathematical form.

The following are the requirements for the application of optimization problems:

- The design or decision variables
- The constraints
- The objective function
- The process model

The Design (Decision) Variables

The first task of optimization process is to identify the underlying design variables that influence the system being optimized.

The design or decision variables are varied during optimization process in order to achieve the optimization goal.

Example: Reactor temperature, Feed rate, No. of plates in a distillation column, Reflux ratio, Batch time, Reactor yield, etc.

The Design (Decision) Variables

A practical problem may involve many design variables.

Some of these may be highly sensitive and heavily influence the process being optimized. Choose these as design variables and others (not so sensitive variables) may be kept constant.

NOTE: If all the design variables are fixed, there is no scope for optimization. Thus one or more variables must be relaxed so that the system becomes an underdetermined system which has, at least in principle, infinite number of solutions.

The Objective Function

A suitable objective function (cost function) is defined in terms of design (or decision) variables and other problem (or process) parameters.

The objective function may be technical or economic, which needs to be either maximized or minimized.

Examples of economic objectives: maximize profits, minimize costs of production.

Examples of technical objectives: maximize reactor yield, minimize size of an equipment, minimize error during curve fitting, minimize environmental impact, etc.

Technical objectives are ultimately related to economics.

The Objective Function

Travel plan for a long trip:

Single objective?

Minimize $f = f_1(x)$

Minimize $f = f_2(x)$

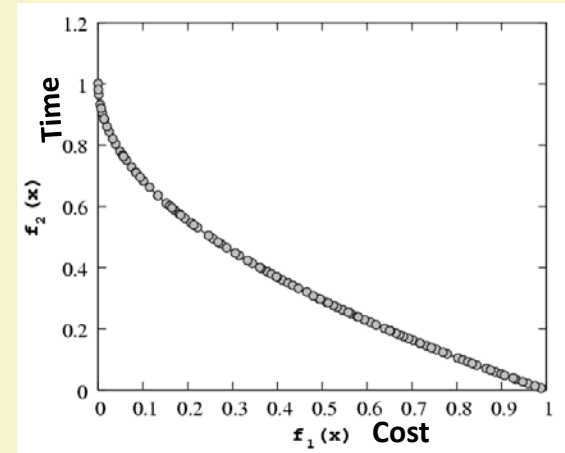
- Minimize ticket price, f_1
- Minimize travel time, f_2

Multiple objectives?

Minimize $f = w_1 f_1(x) + w_2 f_2(x)$
($w_1 + w_2 = 1.0$)

weighting method

Specialized
algorithms are
available for
multi-objective
optimization –
such as Genetic
Algorithms



The Constraints

The constraints represent some additional functional relationships among the decision variables and process parameters. The constraints originate as decision variables must satisfy certain physical phenomenon and certain resource limitations.

Examples:

Variable bounds: $0 \leq x \leq 1$

Equality constraint: Sum of mole fractions should be unity
Component balance equation in distillation column, blending process

Inequality constraints:

In packed bed reactor, temperature should be less than catalyst deactivation temperature
Stress developed anywhere in a component should be less than maximum allowable stress
Acidic condition: $\text{pH} < 7$

The Process Model

A process model is required that describes the manner in which the decision variables are related. The process model also tells us how the objective function is influenced by the decision variables.

A model is a mathematical equation or is a collection of several equations that define how the decision variables are related and the acceptable values these variables can take.

Optimization studies are carried out using a simplified (but reasonably accurate!) model of a real system. Working with real system is time consuming, expensive, risky.

Problem Statement

Given a design vector: $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$

An objective function, $f(\mathbf{x})$

A set of inequality constraints, $\mathbf{g}(\mathbf{x}) \geq 0$

A set of equality constraints, $\mathbf{h}(\mathbf{x}) = 0$

The general problem statement:

$$\begin{aligned} & \min_{\mathbf{x}} f(\mathbf{x}) \\ & \text{subject to} \quad \mathbf{g}(\mathbf{x}) \geq 0 \\ & \quad \quad \quad \mathbf{h}(\mathbf{x}) = 0 \\ & \quad \quad \quad LB \leq \mathbf{x} \leq UB \end{aligned}$$

The optimization problem is to:

“find values of the decision variables that minimize or maximize the objective function while satisfying the constraints.”

Problem Statement

Given a design vector: $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$

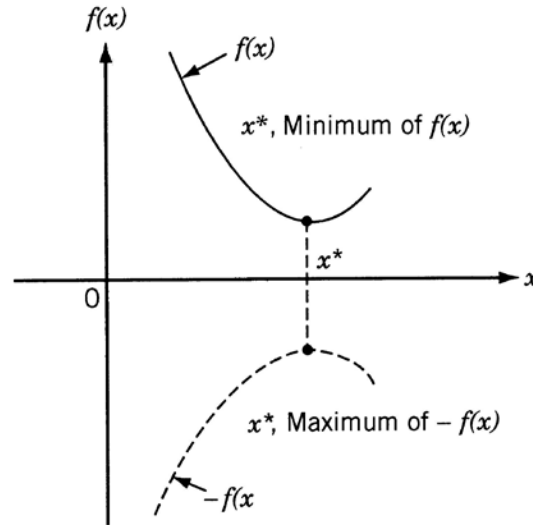
$$\begin{array}{ll}\min_{\mathbf{x}} & f(\mathbf{x}) \\ \text{subject to} & \mathbf{g}(\mathbf{x}) \geq 0 \\ & \mathbf{h}(\mathbf{x}) = 0 \\ & LB \leq \mathbf{x} \leq UB\end{array}$$



$$\begin{array}{ll}\max_{\mathbf{x}} & -f(\mathbf{x}) \\ \text{subject to} & \mathbf{g}(\mathbf{x}) \geq 0 \\ & \mathbf{h}(\mathbf{x}) = 0 \\ & LB \leq \mathbf{x} \leq UB\end{array}$$

Equivalent

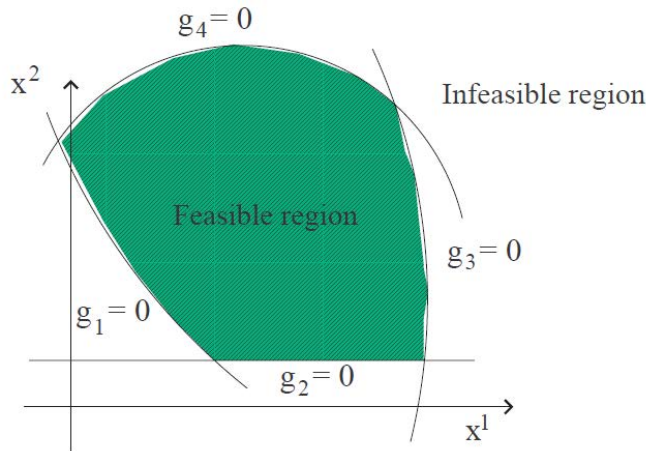
Minimization Vs Maximization



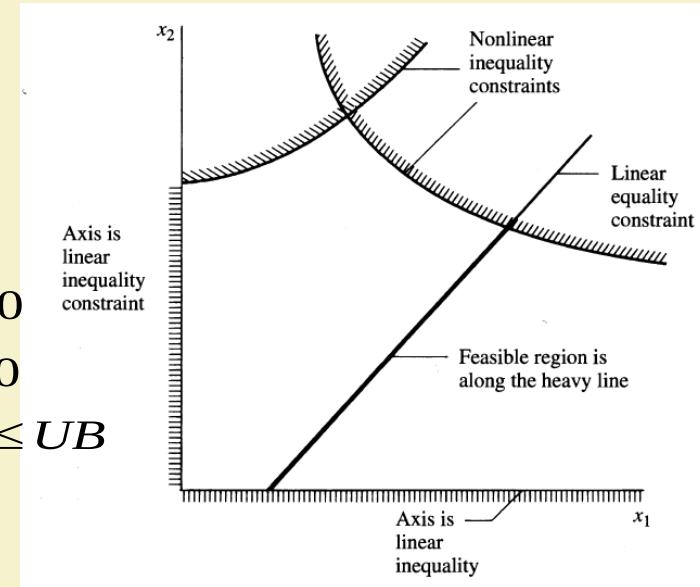
Minimum of $f(x)$ is same as maximum of $-f(x)$.

Constraint Surface

The set of values of $\mathbf{x}$ that satisfy the equation $g(\mathbf{x}) = 0$ forms a hyper-surface in the design space and is called a constraint surface.



$$\begin{aligned} \min_{\mathbf{x}} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{g}(\mathbf{x}) \geq 0 \\ & \mathbf{h}(\mathbf{x}) = 0 \\ & LB \leq \mathbf{x} \leq UB \end{aligned}$$



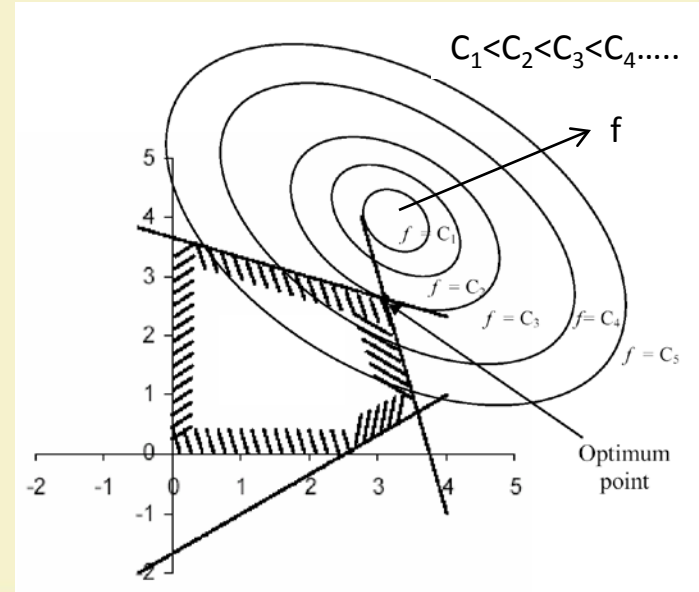
Objective Function Surface

The locus of all points satisfying $f(\mathbf{x}) = C$ (where C is a constant) forms a hyper-surface in the design space and is called objective function surface.

Note: Different values of the constant C will form a family of hyper-surfaces.

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

$$\text{subject to } \mathbf{g}(\mathbf{x}) \geq 0$$
$$\mathbf{h}(\mathbf{x}) = 0$$



Classification of Optimization Methods

Classification based on presence/absence of constraints:

Constrained optimization problems: which are subject to one or more constraints.

Unconstrained optimization problems: in which no constraint exists.

Classification based on the nature of the equations involved:

Linear programming (LP), Nonlinear programming (NLP), Quadratic programming (QP)

Classification based on the nature of the decision variables:

Continuous optimization, Integer programming (IP), MILP, MINLP

Classification of Optimization Methods

Classification based on search space:

Local search methods, Global search methods

Classification based on the number of objective functions:

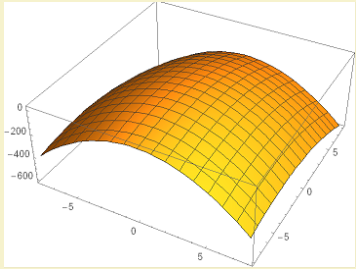
Single objective optimization, Multi-objective optimization

Another Classification:

Deterministic optimization, Stochastic optimization

Optimization in Chemical Engineering

Thank You





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Introduction to Optimization

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Introduction to Optimization

Week 1:



☐ Introduction



☐ Statement of optimization problems



☐ Classification of optimization problems

☐ Examples of engineering applications

☐ Review of linear algebra

Today's Topic:

☐ Examples of engineering applications

Applications of Optimization in Engineering

Theory of optimization finds applications in all branches of engineering. The areas of applications may be broadly divided as follows:

1. Design of system component or entire system
2. Planning and analysis of existing operations
3. Engineering analysis and data reduction
4. Control of dynamic systems: Optimal control/dynamic optimization

Optimal Design of a Can

Design a can which will hold at least 500 ml of liquid. The ranges of height and radius are given as: Height = [7 12] cm, Radius = [3 7] cm

What dimensions for the cylindrical can will use the least amount of material?

We can minimize the material by minimizing the area, A

Objective function:

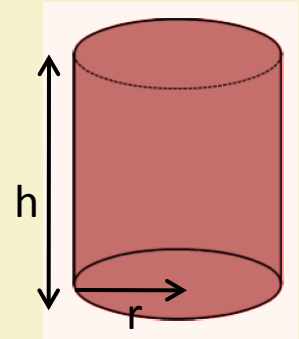
$$A = \underbrace{2\pi r^2}_{\text{area of two ends}} + \underbrace{2\pi rh}_{\text{lateral area}}$$

Constraint:

$$V = \pi r^2 h \geq 500 \text{ ml}$$

Bounds:

$$3 \leq r \leq 7, \quad 7 \leq h \leq 12$$



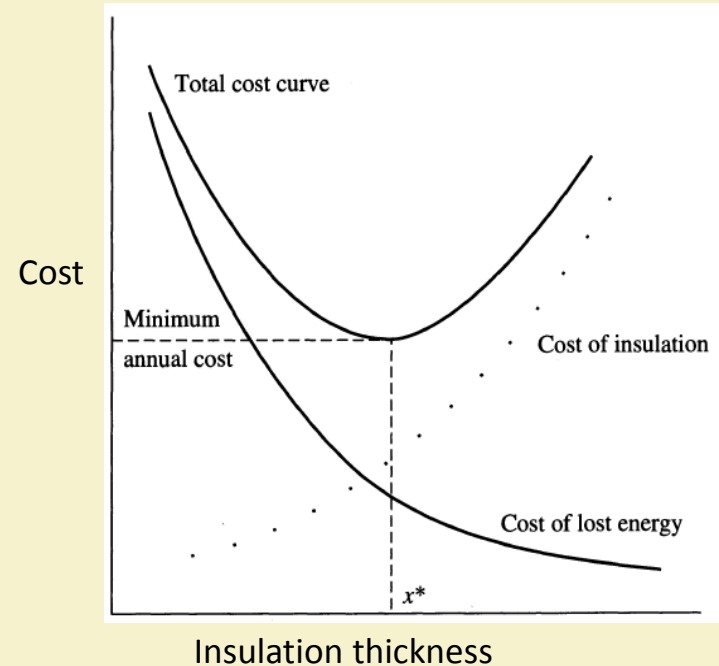
The Optimal Insulation Thickness

Economic criterion:

The addition of insulation should save money through reduced heat losses.

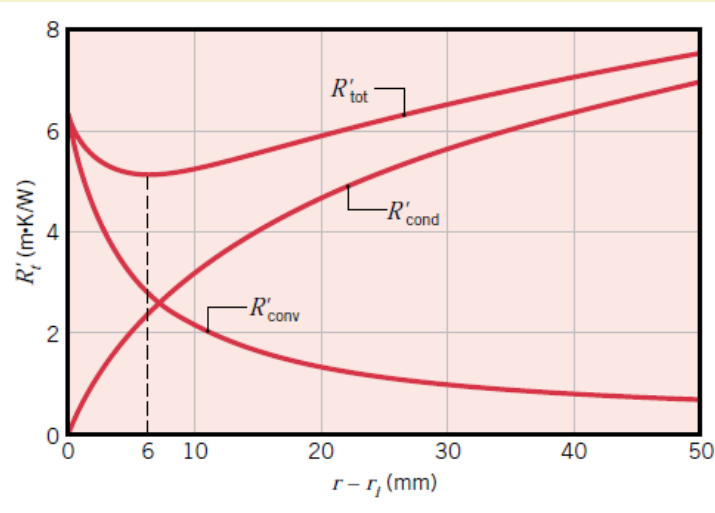
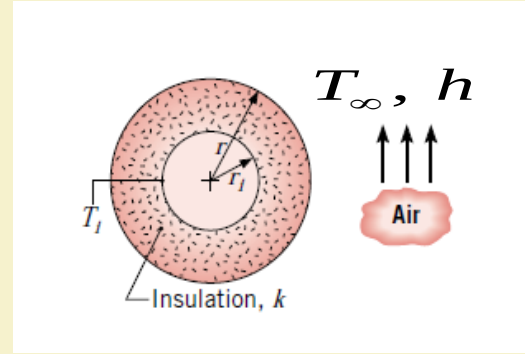
But the insulation material can be expensive.

The optimal amount of insulation needed can be determined by an optimization technique.



The Critical Insulation Thickness

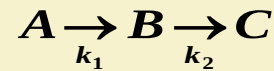
Technical criterion:



$$R_{\text{tot}} = \frac{\ln\left(\frac{r}{r_i}\right)}{2\pi kL} + \frac{1}{(2\pi rL)h}$$

The conduction resistance (first term) increases with the addition of insulation. But the convection resistance (second term) decreases due to increasing outer surface area.

Chemical Reactor Design: Series Reaction

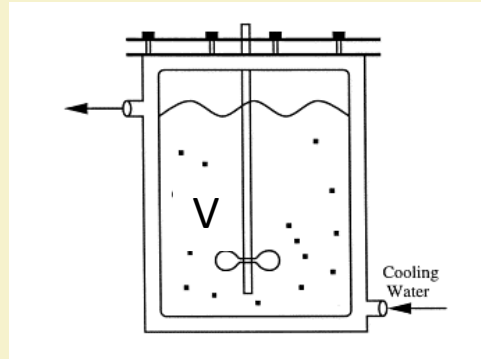


$$k_1 = k_{10} e^{-E_1/RT}$$

$$k_2 = k_{20} e^{-E_2/RT}$$

How to maximize $C_B(t_f)$?

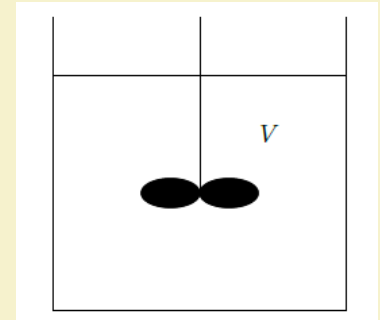
Material Balances:



$$\frac{dC_A}{dt} = -k_1 C_A$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$

$$\frac{dC_C}{dt} = k_2 C_B$$



Energy Balance:

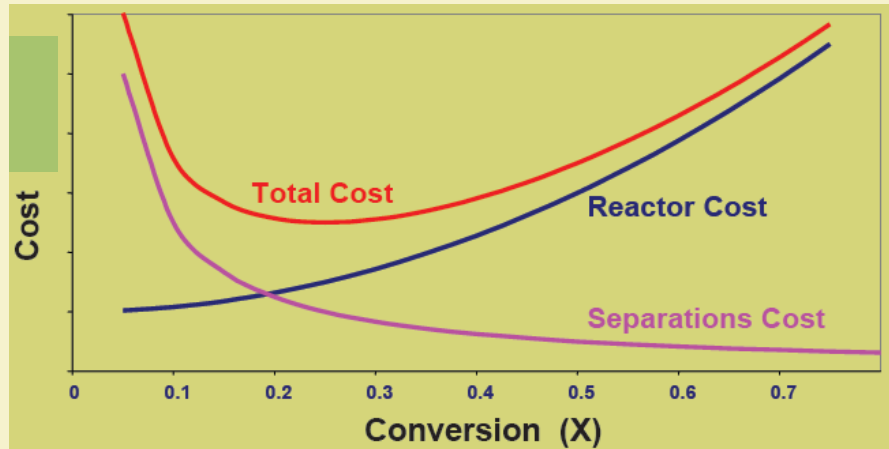
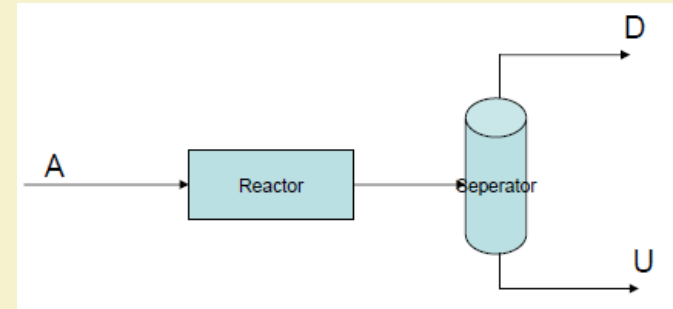
$$\rho V C_P \frac{dT}{dt} = (-\Delta H_1) k_1 C_A V + (-\Delta H_2) k_2 C_B V - UA(T - T_J)$$

Chemical Reactor: Parallel Reaction

Let's look at a reactant, which can form a desired product D, and an undesired side-product U in parallel reactions.



undesired side-product usually needs to be separated



Higher conversion to D will reduce the separation cost, but increases the cost of reactor. What is the optimum conversion?

Refinery Blending Problem

Petrol Type	Octane Rating	Price (INR/liter)
Premium	93	85
Regular	85	80

How much of “Premium Petrol” and how much of “Regular Petrol” should be produced to maximize the profit?

Raw Oil	Octane Rating	Price (INR/liter)	Availability (kilo liter)
1	70	40	200
2	80	50	450
3	85	60	450
4	90	70	500
5	99	75	350

X_{ij} = liter of type i raw oil to make type j petrol

This is an example of Linear Programming Problem.

Diet Problem

Feed	Calories (per 100 g)	Mineral (unit per 100 g)	Vitamin (unit per 100 g)	Cost (INR per 100 g)
Oat	400	50	50	10
Corn	100	100	25	20
Daily minimum Requirement	2000	1000	5000	

Prepare a food mix so that daily requirement is satisfied.

How many gm of Oat and Corn should be fed to minimize the cost?

Nonlinear Regression

Redlich-Kwong equation:
$$P = \frac{RT}{v-b} - \frac{a}{T^{1/2}v(v+b)}$$

From a series of available experimental P-V-T data for a particular gas, find the unknown constants a and b by nonlinear regression for that gas.

Expt. No.	T (K)	V (cc/g mol)	P (atm)
1	273	500	32
2	325	500	42
3	373	600	45
N	370	700	40

Minimize the objective function to find a and b:

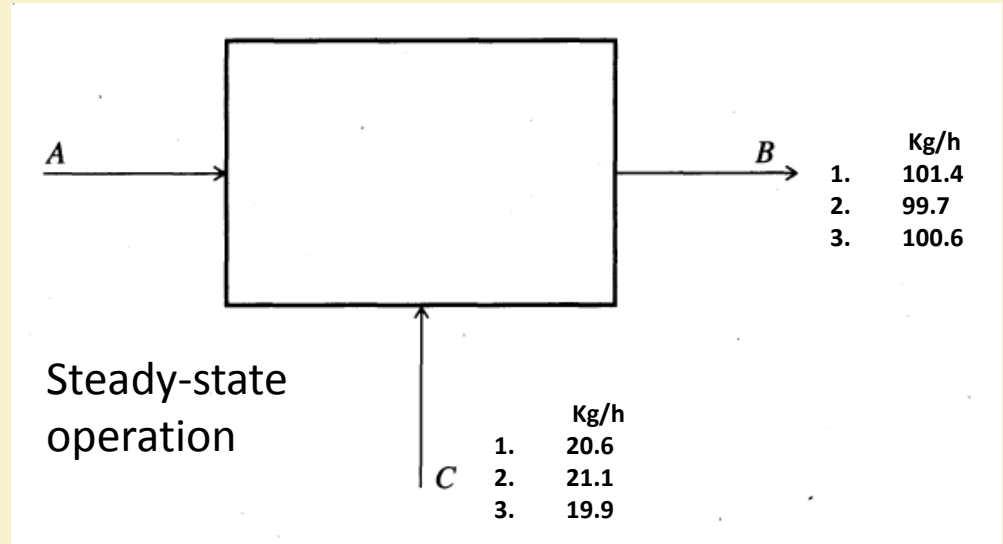
$$\text{Error} = \sum_{i=1}^N \left(P_{i,\text{expt}} - P_{i,\text{calc}} \right)^2$$

The Material Balance Reconciliation

Suppose the flow rates entering and leaving a process are measured periodically. Determine the best value for stream A in kg/h from the three hourly measurements of B and C.

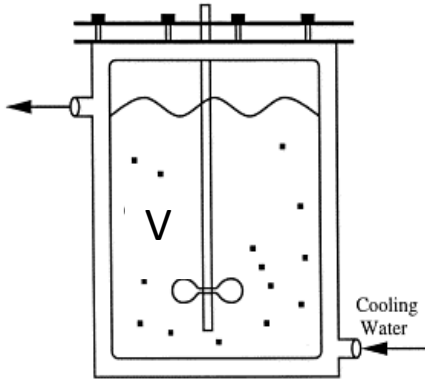
Minimize the objective function to find M_A :

$$\begin{aligned} f(M_A) = & (M_A + 20.6 - 101.4)^2 + \\ & (M_A + 21.1 - 99.7)^2 + \\ & (M_A + 19.9 - 100.6)^2 \end{aligned}$$



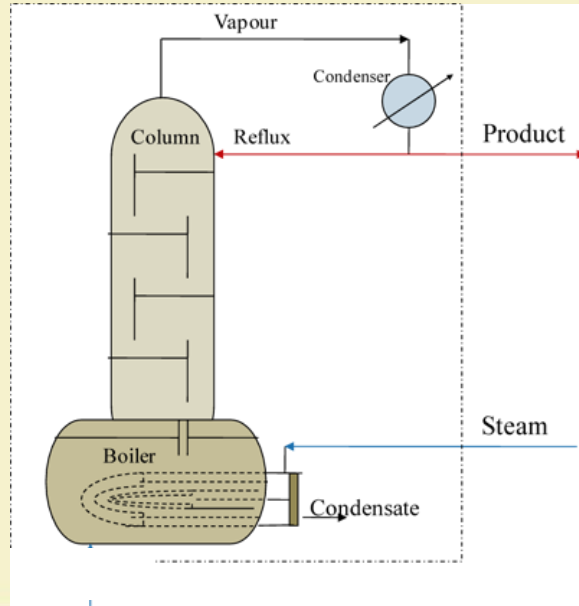
Control of Dynamic Systems: Optimal Control Problem/Dynamic Optimization: Optimal Reactor Temperature

Consider a well-mixed batch reactor where species A and B react to form a product C. The reaction depends on the reactor temperature which can be varied with time.



What should be the temperature profile (temperature versus time function) which maximizes the product concentration at the final time?

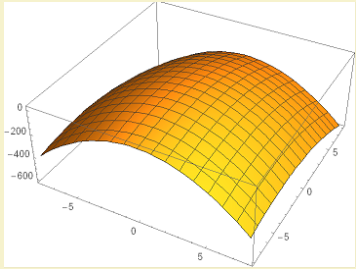
Control of Dynamic Systems: Optimal Control Problem/Dynamic Optimization: Batch Distillation Column



Maximize the production of distillate of a desired purity over a fixed time duration by controlling the distillate production rate with time.

Optimization in Chemical Engineering

Thank You





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Introduction to Optimization

Week 1:



☐ Introduction



☐ Statement of optimization problems



☐ Classification of optimization problems



☐ Examples of engineering applications

☐ Review of linear algebra

Today's Topic:

☐ Review of linear algebra

Vector

Vector is a directed line segment in N-dimensions. It has both “length” and “direction”.

Vector in R^n is an ordered set of n real numbers.

$$\begin{pmatrix} a \\ b \end{pmatrix}^T = (a \quad b)$$

– $v = (1,6,3,4)$ is in R^4

– column vector: $\begin{pmatrix} 1 \\ 6 \\ 3 \\ 4 \end{pmatrix}$

$$\vec{v} = \begin{bmatrix} a \\ b \\ c \end{bmatrix}$$

– row vector: $(1 \quad 6 \quad 3 \quad 4)$

Vector Addition and Vector Subtraction

$$u + v = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} + \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} u_1 + v_1 \\ u_2 + v_2 \end{bmatrix}$$

$$u - v = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} - \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} u_1 - v_1 \\ u_2 - v_2 \end{bmatrix}$$

The difference of two vectors is the result of adding a negative vector

$$\mathbf{A} - \mathbf{B} = \mathbf{A} + (-\mathbf{B})$$

Properties of Vector Addition

1. Commutative: $A+B = B+A$

2. Associative: $(A+B)+C = A+(B+C)$

3. There is a ZERO vector $0 = [0, 0, \dots, 0]^T$ such that
 $A + 0 = 0 + A = A$

Note:

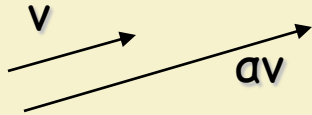
1. $B + (A-B) = A$

2. $-(-B) = B$

3. $-(A-B) = B-A$

Vector Multiplication: By Scalar

$$\alpha \mathbf{v} = \alpha(x_1, x_2) = (\alpha x_1, \alpha x_2)$$



Properties:

- Distributive:**
 $\alpha(A + B) = \alpha A + \alpha B$
 $(\alpha + \beta)A = \alpha A + \beta B$
- Associative:**
 $\alpha(\beta A) = (\alpha\beta)A$

The scalar 1, α , 0, -1 satisfies:

$$1A = A, \quad \alpha 0 = 0,$$

$$0\alpha = 0, \quad (-1)A = -A$$

Linear Combination

Given: vectors $v_1, v_2, \dots, v_n$ in $\mathbb{R}^n$ and n real number $c_1, c_2, \dots, c_n$, the vector x obtained by

$$x = c_1 v_1 + c_2 v_2 + \dots + c_n v_n$$

is called a **linear combination** of $v_1, v_2, \dots, v_n$

Examples of linear combination of v_1 and v_2 :

$$\frac{1}{2}v_1 + \sqrt{5}v_2$$

$$0.5v_2 = 0v_1 + 0.5v_2$$

Linear Independence

A set of vectors $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k\}$ is called **linearly dependent** if there exist scalars $c_1, c_2, \dots, c_k$, not all zero, such that $c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + \dots + c_k\mathbf{v}_k = \mathbf{0}$ (i.e. $\sum_i c_i \mathbf{v}_i = \mathbf{0}$)

The vectors are **linearly independent** if the above equation is satisfied ONLY by

$$c_1 = c_2 = \dots = c_k = 0$$

Examples:

The set $S = \{(1, 2), (3, 4)\}$ is linearly dependent because
 $-2(1, 2) + 1(2, 4) = (0, 0)$

The set $S = \{(1, 0), (0, 1), (-2, 5)\}$ is linearly dependent because
 $2(1, 0) - 5(0, 1) + 1(-2, 5) = (0, 0)$

Linear Independence

Determine whether the following set of vectors is linearly dependent or linearly Independent: $\mathbf{v}_1 = (1, 2, 3)$, $\mathbf{v}_2 = (0, 1, 2)$, $\mathbf{v}_3 = (-2, 0, 1)$

Solution: $c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + c_3\mathbf{v}_3 = \mathbf{0}$

$$\Rightarrow c_1(1, 2, 3) + c_2(0, 1, 2) + c_3(-2, 0, 1) = (0, 0, 0)$$

$$\Rightarrow (c_1 - 2c_3, 2c_1 + c_2, 3c_1 + 2c_2 + c_3) = (0, 0, 0)$$

$$\Rightarrow c_1 = c_2 = c_3 = 0$$

Therefore, the set of vectors is linearly independent.

Linear Independence: Properties

- A set of vectors is linearly dependent if and only if one of the vectors is a linear combination of the others.
- Any set of vectors containing the zero vector is linearly dependent.
- If a set of vectors is linearly independent, then any subset of these vectors is also linearly independent.
- If a set of vectors is linearly dependent, then any larger set, containing this set, is also linearly dependent.

Dot Product (Inner Product, Scalar Product) of Vectors

$$A \cdot B = A^T B = \begin{bmatrix} a & b & c \end{bmatrix} \begin{bmatrix} d \\ e \\ f \end{bmatrix} = ad + be + cf$$

The dot product is a scalar

$$\langle x, y \rangle = \sum_{i=1}^n x_i y_i$$

$$\|A\|^2 = A^T A = aa + bb + cc$$

The magnitude of a vector is the dot product of a vector with itself

$$A \cdot B = \|A\| \|B\| \cos(\theta)$$

The dot product is related to the angle between the two vectors

Inner Product Vs Outer Product

Inner product:
$$u \bullet v = u^T v = \begin{pmatrix} u_1 & u_2 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = u_1 v_1 + u_2 v_2$$

Outer product:
$$uv^T = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \begin{pmatrix} v_1 & v_2 \end{pmatrix} = \begin{pmatrix} u_1 v_1 & u_1 v_2 \\ u_2 v_1 & u_2 v_2 \end{pmatrix}$$

Vector Norms

The norm of a vector is a measure of the magnitude or length of the vector.

$$\|x\|_1 = \sum_{i=1}^n |x_i|$$

1-norm

$$\|x\|_2 = \left(\sum_{i=1}^n |x_i|^2 \right)^{1/2}$$

2-norm

$$\|x\|_\infty = \max_i |x_i|$$

∞ -norm

In general, p-norm:
$$\|x\|_p = \left(\sum_{i=1}^n |x_i|^p \right)^{1/p}$$

Vector Norms: Properties

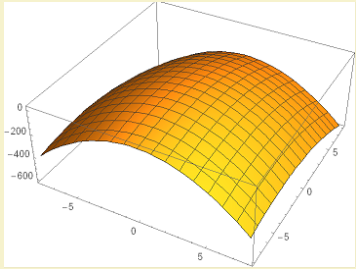
$$\|x\| > 0 \text{ if } x \neq 0$$

$$\|\alpha x\| = |\alpha| \cdot \|x\| \text{ for any scalar } \alpha$$

$$\|x + y\| \leq \|x\| + \|y\| \text{ (triangle inequality)}$$

Optimization in Chemical Engineering

Thank You





IIT KHARAGPUR



NPTEL ONLINE
CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Introduction to Optimization

(WEEK – 1: LECTURE - 5)

Dr. Debasis Sarkar

**Department of Chemical Engineering
Indian Institute of Technology Kharagpur**

Introduction to Optimization

Week 1:



☐ Introduction



☐ Statement of optimization problems



☐ Classification of optimization problems



☐ Examples of engineering applications

☐ Review of linear algebra

Today's Topic:

☐ Review of linear algebra

Matrix Algebra

An $(m \times n)$ matrix, A , is a rectangular array of elements

$$A = [a_{ij}] = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

m = # of rows

n = # of columns

dimensions = $(m \times n)$

Matrix Operations: Addition

Let $A = [a_{ij}]$ and $B = [b_{ij}]$ denote two $(m \times n)$ matrices. Then the sum, $A + B$, is the matrix

$$c_{ij} = a_{ij} + b_{ij} \text{ for } 1 \leq i \leq m, 1 \leq j \leq n$$

$$C = A + B = \begin{bmatrix} a_{11} + b_{11} & a_{12} + b_{12} & \cdots & a_{1n} + b_{1n} \\ a_{21} + b_{21} & a_{22} + b_{22} & \cdots & a_{2n} + b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} + b_{m1} & a_{m2} + b_{m2} & \cdots & a_{mn} + b_{mn} \end{bmatrix}$$

The dimensions of A and B are required to be both $(m \times n)$.

Matrix Operations: Scalar Multiplication

Let $A = (a_{ij})$ denote an $(m \times n)$ matrix and let c be any scalar. Then cA is the matrix

$$cA = (ca_{ij}) = \begin{bmatrix} ca_{11} & ca_{12} & \cdots & ca_{1n} \\ ca_{21} & ca_{22} & \cdots & ca_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ ca_{m1} & ca_{m2} & \cdots & ca_{mn} \end{bmatrix}$$

Matrix Multiplication

Let $A = [a_{ij}]$ denote an $(m \times n)$ matrix and $B = [b_{ij}]$ denote an $(n \times q)$ matrix

Then the product of A and B is an $(m \times q)$ matrix $C = [c_{ij}]$ where

$$c_{ij} = \sum_{k=1}^n a_{ik} b_{kj}$$

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

$$AB = \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{pmatrix}$$

Identity Matrix, Zero Matrix, Symmetric Matrix

An $n \times n$ **identity** matrix, I , is the square matrix:

Note: $AI = A$ and $IA = A$.

$$I = I_n = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

Zero matrix:
(Null matrix)

$$A = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Symmetric matrix: A symmetric matrix is a square matrix which is symmetric about its leading diagonal.

$$B = \begin{bmatrix} 4 & -1 \\ -1 & 9 \end{bmatrix} \quad C = \begin{bmatrix} 2 & 7 & 3 \\ 7 & 9 & 4 \\ 3 & 4 & 7 \end{bmatrix}$$

Diagonal matrix:

$$\begin{bmatrix} a_{11} & 0 & 0 & 0 \\ 0 & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & 0 \\ 0 & 0 & 0 & a_{44} \end{bmatrix}$$

Matrix Operations: Properties

Matrix addition:

$$A + B = B + A$$

$$(A + B) + C = A + (B + C)$$

$$A + \mathbf{0} = \mathbf{0} + A = A$$

Matrix Multiplication:

$$A(BC) = (AB)C$$

$$A(B + C) = AB + AC$$

$$(A + B)C = AC + BC$$

If A is a square matrix of order n

If $p > 0$, $A^p = A.A.A.....A$ p times

and

$$A^0 = I_n$$

The Determinant of a Square Matrix

The determinant of a matrix A is denoted by $|A|$ (or $\det(A)$).

Determinants exist only for square matrices ($n \times n$).

$$|A| = \det \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} = \sum_{j=1}^n a_{ij} A_{ij}$$

$$\det \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

Here, A_{ij} = cofactor of a_{ij} =
 $(-1)^{i+j}$ $\left(\begin{array}{l} \text{the determinant of the matrix} \\ \text{after deleting } i^{th} \text{ row and } j^{th} \text{ col} \end{array} \right)$.

Properties of Determinants

1. $|A| = |A'|$.
2. If a row or column of $A = 0$, then $|A| = 0$.
3. If every value in a row or column is multiplied by k , then $|A| = k|A|$.
4. If two rows or columns are identical, $|A| = 0$.
5. If two rows or columns are linear combination of each other, $|A| = 0$.
6. $|A|$ remains unchanged if each element of a row is multiplied by a constant and added to any other row.
7. $|AB| = |A| |B|$
8. Determinant of a diagonal matrix = product of the diagonal elements

The Transpose of a Matrix

Consider the $(m \times n)$ matrix, $A = [a_{ij}] = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$

Then the $(n \times m)$ matrix, A' (also denoted by A^T) is called the transpose of A .

$$A' = [a_{ji}] = \begin{bmatrix} a_{11} & a_{21} & \cdots & a_{m1} \\ a_{12} & a_{22} & \cdots & a_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{mn} \end{bmatrix}$$

An $(n \times n)$ matrix,
 A , is said to be
symmetric if
 $A' = A$

$$\begin{aligned} (AB)' &= B'A' \\ (AB)^{-1} &= B^{-1}A^{-1} \\ (A')^{-1} &= (A^{-1})' \end{aligned}$$

Inverse of a Matrix

Let A denote the $(n \times n)$ matrix.

Let B denote an $(n \times n)$ matrix such that $AB = BA = I$.

If the matrix B exists then A is called **invertible**. Also B is called the **inverse** of A and is denoted by A^{-1}

Let A and B be two matrices whose inverse exists. Let $C = AB$. Then the inverse of the matrix C exists and $C^{-1} = B^{-1}A^{-1}$.

Inverse of a Matrix

1. The inverse (A^{-1}) is defined such that $A A^{-1}$ is I. Not every matrix has an inverse. If no inverse exists, then the matrix is called singular (non invertible, $\text{Det} = 0$)
2. If A is nonsingular, then A^{-1} is also nonsingular.
3. If A, B are nonsingular, then AB is also non singular and $(AB)^{-1} = B^{-1}A^{-1}$
4. $(ABC)^{-1} = C^{-1}B^{-1}A^{-1}$
5. If A is nonsingular, then its transpose is also nonsingular. Also, $(A^T)^{-1} = (A^{-1})^T$

Rank of a Matrix

The rank of a matrix is defined as

$\text{rank}(\mathbf{A})$ = the number of linearly independent rows
= the number of linearly independent columns

If a matrix $\mathbf{A}$ of dimension $m \times n$ (where $n < m$) is of rank n , then $\mathbf{A}$ has maximum possible rank and is said to be of full rank.

$r(O)=0$. As long as A is not 0, $r(A) > 0$.

In general, the maximum possible rank of an $(m \times n)$ matrix $\mathbf{A}$ is $\min(m, n)$.

Elementary Row and Column Operations

The following elementary row or column operations yield an equivalent system:

- Interchanges: Two rows (or columns) can be interchanged
- Scaling: Multiplying a row (or column) by a nonzero constant
- Sum: The row (or column) can be replaced by the sum of that row (column) and a nonzero multiple of any other row (column).

Elementary operations do not change the rank. One can use ERO and ECO to find the rank of a matrix as follows:

ERO $\Rightarrow$ minimum # of rows with at least one nonzero entry

ECO $\Rightarrow$ minimum # of columns with at least one nonzero entry

Linear Systems in Matrix Form

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\ \vdots & \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n &= b_n \end{aligned} \quad \Rightarrow \quad \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

The linear system of equations $A \cdot x = b$ has a solution, or said to be consistent if $\text{Rank}\{A\} = \text{Rank}\{A|b\}$

A system is inconsistent when $\text{Rank}\{A\} < \text{Rank}\{A|b\}$

The system has a unique solution if: $\text{Rank}\{A\} = \text{Rank}\{A|b\} = n$ where n is the order of the system.

$$A \cdot \vec{x} = \vec{b}$$

$$A^{-1}A \cdot \vec{x} = A^{-1}\vec{b}$$

$$\vec{x} = A^{-1}\vec{b}$$

Gaussian Elimination

- By using Elementary Row Operations (ERO), matrix A is transformed into an upper triangular matrix (all elements below diagonal are 0)
- Back substitution is used to solve the upper-triangular system

$$\begin{bmatrix} a_{11} & \cdots & a_{1i} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots & & \vdots \\ a_{i1} & \cdots & a_{ii} & \cdots & a_{in} \\ \vdots & & \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{ni} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_i \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_i \\ \vdots \\ b_n \end{bmatrix} \xRightarrow{\text{ERO}} \begin{bmatrix} a_{11} & \cdots & a_{1i} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots & & \vdots \\ 0 & \cdots & \tilde{a}_{ii} & \cdots & \tilde{a}_{in} \\ \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & \tilde{a}_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_i \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ \tilde{b}_i \\ \vdots \\ \tilde{b}_n \end{bmatrix}$$



Back substitution

Gaussian Elimination

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

Divide Row 1 by 25 and multiply by 64. Subtract the result from Row 2.

Repeat such steps to get upper triangular matrix.



$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.21 \\ 0.735 \end{bmatrix}$$

Eigenvalues, Eigenvectors of a Matrix

Let A be an $n \times n$ matrix. Let $\vec{x}$ and λ be such that

$$A\vec{x} = \lambda\vec{x} \quad \text{with } \vec{x} \neq \vec{0}$$

then λ is called an eigenvalue of A and $\vec{x}$ is called an eigenvector of A .

Note: $(A - \lambda I)\vec{x} = \vec{0}$ thus $|A - \lambda I| = 0$ is the condition for an eigenvalue.

$$|A - \lambda I| = \det \begin{bmatrix} (a_{11} - \lambda) & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \cdots & (a_{nn} - \lambda) \end{bmatrix} = 0$$

Here, the det is a polynomial of degree n in λ .

Thus, there are n possible eigenvalues $\lambda_1, \dots, \lambda_n$

Optimization in Chemical Engineering

Thank You

