



IIT KHARAGPUR



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CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Optimization Problem Formulation

(WEEK – 2: LECTURE - 6)

Dr. Debasis Sarkar

Department of Chemical Engineering
Indian Institute of Technology Kharagpur

Optimization Problem Formulation

Week 2:

- ☐ Models for optimization
- ☐ Degrees of freedom analysis
- ☐ Optimization problems in chemical/biochemical engineering

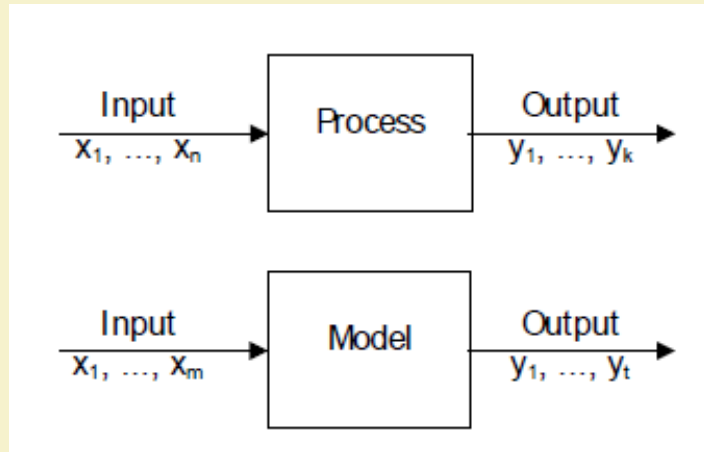
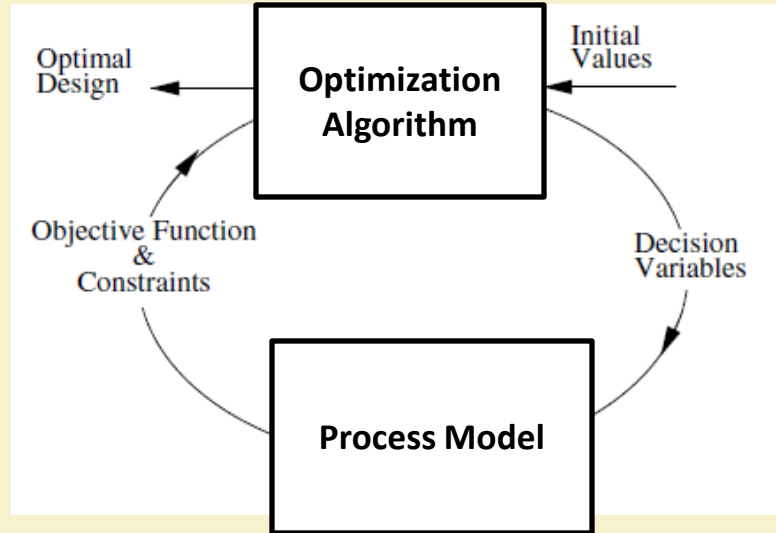
Process Models for Optimization

Optimization requires use of mathematical techniques for maximization or minimization of an objective function. With advent of computers, optimization have become part of computer-aided design activities.

In order to use optimization algorithms on computers, we must have a quantitative model available to compute the responses of interest and objective function. If we wish to maximize heat transfer from a fin, we must be able to calculate the amount of heat transfer for different designs of fin. If we wish to minimize cost, we must be able to calculate cost. During heat exchanger design, if pressure drop can not exceed 10 psi (say), we must be able to compute pressure drop given shell/tube pass, number of baffles, etc.

Getting a valid, accurate model of the process is an important step in optimization.

Process Models for Optimization



Process Models for Optimization

In an optimization problem, constraints arise because a process must describe the physical bounds on the design variables, empirical relations among design variables, and physical laws that apply to a specific problem.

To optimize a process, we need a process model to formulate the objective function, equality constraints, and inequality constraints .

A process model is a set of equations that imitates reality and cannot incorporate all features of the real process. However, a reasonably accurate model saves us time and money as we can avoid repetitive experimentation and measurements.

Remember: Quality of optimal solution depends on accuracy of the process model used.

Classification of Process Models

Broadly two types:

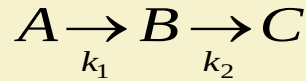
- ❑ Models based on physical theory (uses physical, chemical laws. First-principle based models)
- ❑ Models based on strictly empirical descriptions (black box models, data based models).

Other types of models:

- Linear versus nonlinear.
- Steady state versus unsteady state.
- Lumped parameter versus distributed parameter.
- Continuous versus discrete variables.

Series Reaction Optimization: Theoretical Model

Material Balances:



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

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

How to maximize $C_B(t_f)$?

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

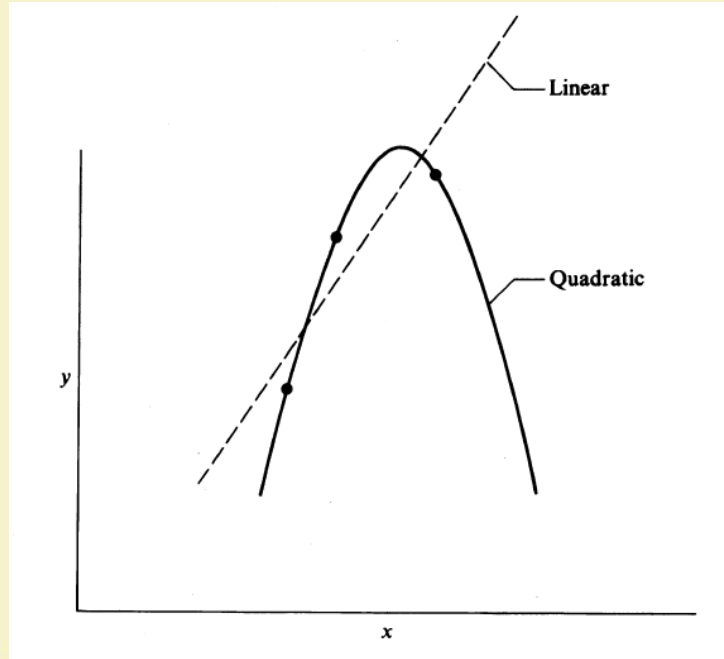
$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$

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

Energy Balance:

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

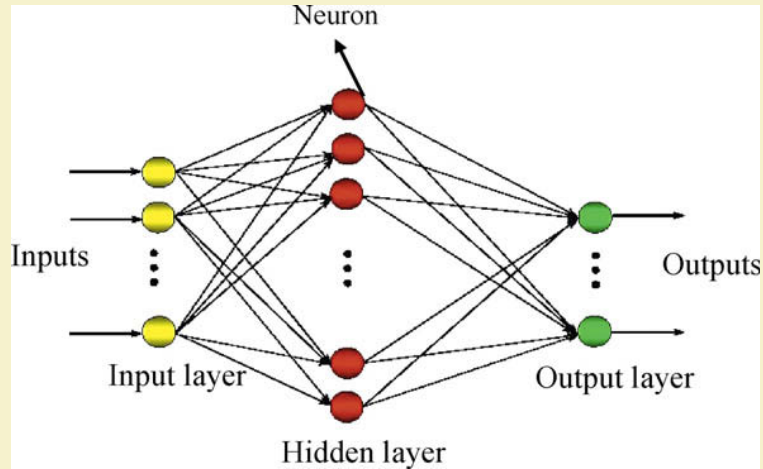
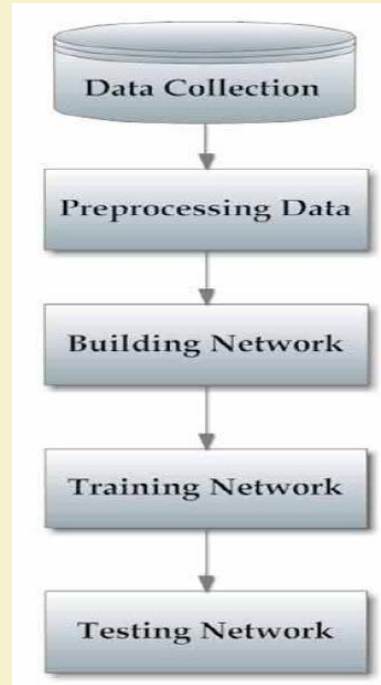
Empirical Model: Regression



Linear: $y = \alpha + \beta x$

Quadratic: $y = \alpha_1 + \alpha_2 x + \alpha_3 x^2$

Empirical Model: Neural Network



The Degrees of Freedom Analysis

The degrees of freedom analysis gives us the number of decision variables that can be changed during optimization process to obtain the optimal solution.

Degrees of freedom, $DOF = (\text{No. of variables}) - (\text{No. of linearly independent equations})$

If $DOF = 0$, unique solution exists. No optimization is possible.

If $DOF > 0$, under-determined system. Infinite solutions exist. Optimization possible.

If $DOF < 0$, over-determined system. No solution exists. Least square analysis possible.

$$\text{Min } x_1^2 + x_2^2$$

subject to:

$$x_1 - x_2 = 6$$

$$x_1 + x_2 = 2$$

$$\text{Min } x_1^2 + x_2^2$$

subject to:

$$x_1 - x_2 = 6$$

$$\text{Min } x_1^2 + x_2^2$$

subject to:

$$x_1 - x_2 \leq 6$$

$$x_1 + x_2 \leq 2$$

The Degrees of Freedom (DOF) Analysis: Example

Minimize: $f(x) = 4x_1 - x_2^2 - 12$

Subject to: $25 - x_1^2 - x_2^2 = 0$

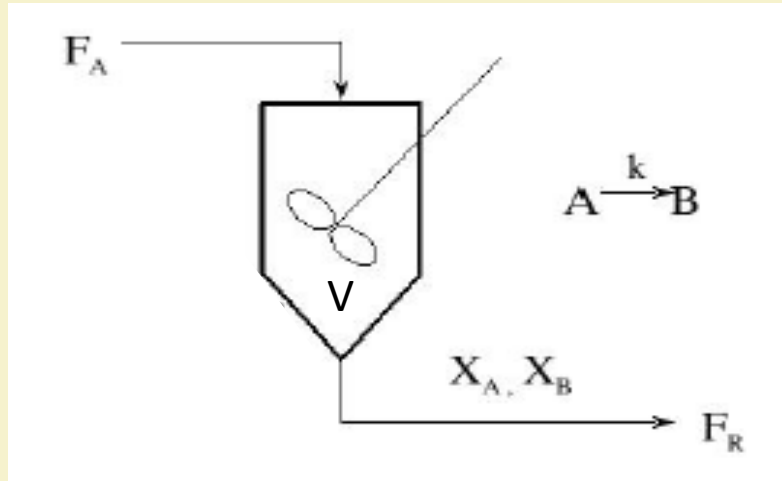
$$10x_1 - x_1^2 + 10x_2 - x_2^2 - 34 \geq 0$$

$$(x_1 - 3)^2 + (x_2 - 1)^2 \geq 0$$

$$x_1, x_2 \geq 0$$

1. How many variables are there?
2. How many independent variables are there?
3. What is the DOF?

The Degrees of Freedom (DOF) Analysis: Another Example



mass		$F_A - F_R = 0$
component A		$F_A - kX_A V \rho - X_A F_R = 0$
component B		$kX_A V \rho - X_B F_R = 0$

$1 - X_A - X_B = 0$

If we specify: F_A , V , ρ , k

We have 3 variables (X_A , X_B , F_R) and 4 Eq.

Are all equations linearly independent?

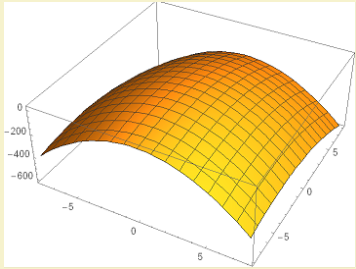
Perform: (Component A + Component B) – Mass

Only 3 linearly independent equations.

DOF = 0

Optimization in Chemical Engineering

Thank You





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Optimization Problem Formulation

(WEEK – 2: LECTURE - 7)

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Optimization Problem Formulation

Week 2:

-  ☐ Models for optimization
-  ☐ Degrees of freedom analysis
- ☐ Optimization problems in chemical/biochemical engineering

General Problem Formulation

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:

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

Optimization Problem Formulation: Understand the Problem

Example:

A manufacturer produces a chemical Q from two raw materials: R_1 and R_2 . Cost of R_1 is Rs. 100 per kg and cost of R_2 is Rs. 50 per kg. Determine the amount of each raw material required to minimize the cost of product Q per kg.

Optimal Design of a Can: The Problem

A cylindrical can with volume at least V_0 is to be designed in such a way as to minimize the total cost of the material in a box of 12 cans, arranged in a 3×4 pattern.

The cost is proportional to surface area of cans and box. It is given as

$$\text{Cost} = c_1 S_1 + c_2 S_2$$

where S_1 is the surface area of the 12 cans and S_2 is the surface area of the box. The constant coefficients c_1 and c_2 are positive.

Another constraint is that no dimension of the box can exceed a given value D_0 .

Optimal Design of a Can: Formulation

design parameters: r = radius of can, h = height of can

volume constraint: $\pi r^2 h \geq V_0$

surface area of cans: $S_1 = 12(2\pi r^2 + 2\pi rh) = 24\pi r(r + h)$

box dimensions: $8r \times 6r \times h$

surface area of box: $S_2 = 2(48r^2 + 8rh + 6rh) = 4r(24r + 7h)$

size constraints: $8r \leq D_0$, $6r \leq D_0$, $h \leq D_0$

nonnegativity constraints: $r \geq 0$, $h \geq 0$

The cost function is:

$$f(r, h) = c_1[24\pi r(r + h)] + c_2[4r(24r + 7h)]$$

$$\text{Min } f(r, h)$$

subject to:

$$\pi r^2 h \geq V_0$$

$$8r \leq D_0, 6r \leq D_0, h \leq D_0$$

$$r \geq 0, h \geq 0$$

Chemical Equilibrium by Gibbs Energy Minimization

Ethane reacts with steam in presence of a catalyst to form hydrogen at 1000 °C temperature and 1 atm pressure. The feed contains 4 moles of steam per mole of ethane. At equilibrium, the following compounds are present in the mixture:

CH ₄	4.61
C ₂ H ₄	28.249
C ₂ H ₂	40.604
CO ₂	-94.61
CO	-47.942
O ₂	0
H ₂	0
H ₂ O	-46.03
C ₂ H ₆	26.13

The Gibbs energy of formation for the compounds present in the mixture are also known at the given reaction condition and shown here next to the compound.

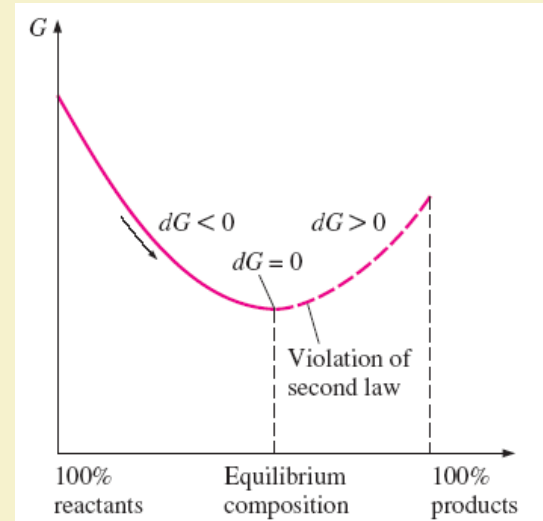
How to determine the composition of the equilibrium mixture?

Chemical Equilibrium by Gibbs Energy Minimization

Problem: Determine the composition of a reacting mixture at equilibrium.

A chemical reaction at a specified temperature and pressure proceeds in the direction of a decreasing Gibbs free energy. The reaction stops and chemical equilibrium is established when the Gibbs free energy attains a minimum value.

Therefore, the composition of a reacting mixture at chemical equilibrium can be determined by formulating a problem that minimizes Gibbs free energy, with atom balance as constraint.



Criteria for chemical equilibrium for a fixed mass at a specified temperature and pressure.

Chemical Equilibrium by Gibbs Energy Minimization

Let us consider a reacting mixture at equilibrium with m number of elements and n number of compounds.

Let us define,

$x(j)$ = number of moles for compound j , $j = 1, 2, \dots, n$

v_{ij} = number of atoms of element i in a molecule of compound j

w_i = atomic weight of element i , $i = 1, 2, \dots, m$

Chemical Equilibrium by Gibbs Energy Minimization

$$\text{Min}_x f(x) = \sum_{j=1}^n x_j \left[\frac{G_j^0}{RT} + \ln(P) + \ln \frac{x_j}{\sum_{j=1}^n x_j} \right]$$

Gibbs free energy function.

Here G_j^0 is the Gibbs free energy of pure component j .

R is the gas constant.

subject to:

$$\sum_{j=1}^n \nu_{ij} x_j = w_i, \quad i = 1, \dots, m$$

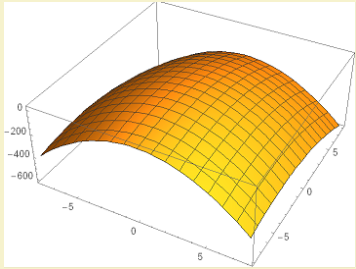
Atom balance constraint

$$x_j \geq 0, \quad j = 1, \dots, m$$

Non-negativity constraint on number of moles

Optimization in Chemical Engineering

Thank You





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(WEEK – 2: LECTURE - 8)

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Optimization Problem Formulation

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- ☐ Optimization problems in chemical/biochemical engineering

General Problem Formulation: Review

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:

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

Optimization Problem Formulation: Product Mix

A food company decides to produce two new soft-drinks: Drink-1 and Drink-2. The company has 3 plants.

Production time needed for each unit produced			
Plant	Drink-1	Drink-2	Availability/week
1	1 hour	0	4 hours
2	0	2 hours	12 hours
3	3 hours	2 hours	18 hours

Unit profit for Drink-1 is Rs. 3 and unit profit for Drink-2 is Rs. 5. How many of each item should be produced weekly to maximize the profit?

Optimization Problem Formulation: Product Mix

Production time used
for each unit produced

Plant	Drink-1	Drink-2	Availability/week
1	1 hour	0	4 hours
2	0	2 hours	12 hours
3	3 hours	2 hours	18 hours

Decision variables:

x = No. of Drink-1 produced per week,

y = No. of Drink-2 produced per week

$$\text{Max}_{x,y} f(x,y) = 3x + 5y$$

subject to

$$x \leq 4$$

$$2y \leq 12$$

$$3x + 2y \leq 18$$

$$x \geq 0, y \geq 0$$

We are maximizing weekly profit.

Another Example on Product Mix

A fertilizer manufacturing company produces two types of fertilizer: Type A: having high phosphorus content, and Type B: having low phosphorus content.

Raw Material	Tons required per ton of fertilizer		Maximum availability per day, ton
	Type A	Type B	
Urea	2	1	3000
Potash	1	1	2400
Rock phosphate	1	0	1000
Net profit per ton	30	20	

What should be the daily production schedule (tons of A and B produced) to maximize the profit?

Decision variables:

Daily production of Type A: x tons, Type B: y tons

The objective function:

Maximize profit, $z = 30x + 20y$

Another Example on Product Mix

Raw Material	Tons required per ton of fertilizer		Maximum availability per day
	Type A	Type B	
Urea	2	1	3000
Potash	1	1	2400
Rock phosphate	1	0	1000
Net profit per ton	30	20	

Maximize $z(x, y) = 30x + 20y$
 subject to $2x + y \leq 3000$
 $x + y \leq 2400$
 $x \leq 1000$
 $x \geq 0,$
 $y \geq 0$

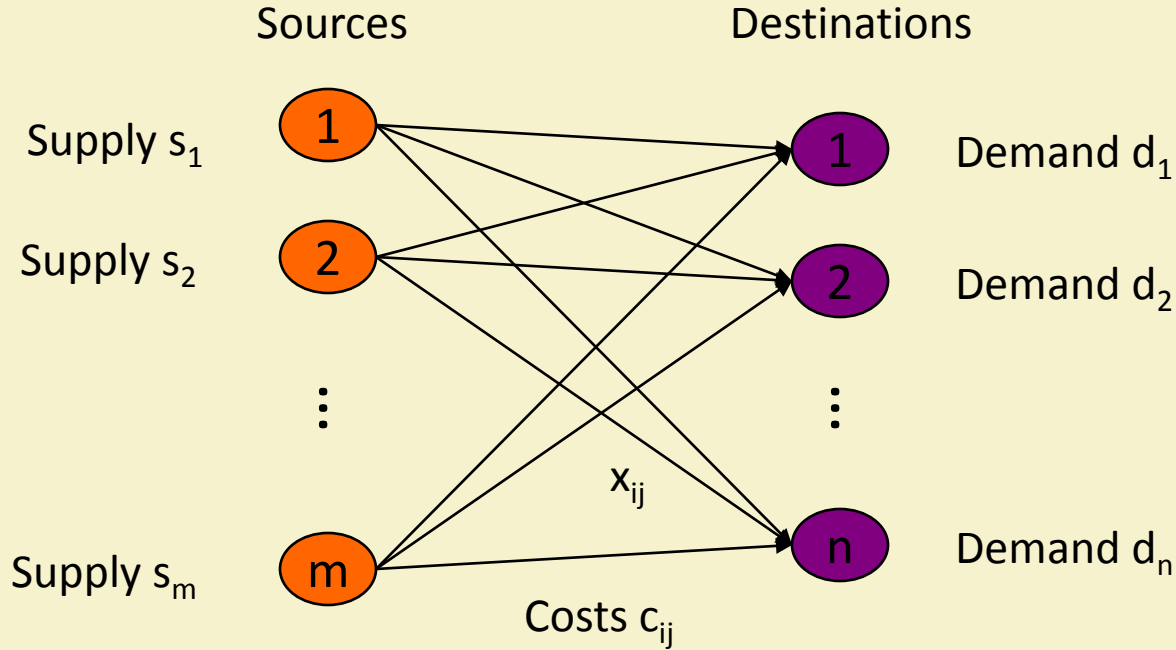
The Transportation Problem

In a Transportation Problem, we wish to find the minimum-cost distribution of a given commodity from a group ($i = 1, \dots, m$) of supply centers (sources) to a group ($j = 1, \dots, n$) of receiving centers (destinations).

Each source has a certain supply (s_i). Each destination has a certain demand (d_j).

The cost of shipping from a source to a destination is directly proportional to the number of units shipped.

A Simple Transport Network Representation



The Transportation Problem

	Warehouse					
Factory	A	B	C	D	Supply	
1	4	7	7	1	100	
2	12	3	8	8	200	Total Supply
3	8	10	16	5	150	
Demand	80	90	120	160		450
			Total Demand		450	

Minimize the total shipping cost.

Let $x_{i,j}$ be the quantity shipped from factory i to warehouse j .

$$\begin{aligned} \text{Minimize } & \left(4x_{1,A} + 7x_{1,B} + 7x_{1,C} + x_{1,D} \right) + \left(12x_{2,A} + 3x_{2,B} + 8x_{2,C} + 8x_{2,D} \right) + \\ & \left(8x_{3,A} + 10x_{3,B} + 16x_{3,C} + 5x_{3,D} \right) \end{aligned}$$

The Transportation Problem

	Warehouse					
Factory	A	B	C	D	Supply	
1	4	7	7	1	100	Total Supply
2	12	3	8	8	200	
3	8	10	16	5	150	
Demand	80	90	120	160		450
			Total Demand		450	

Let $x_{i,j}$ be the quantity shipped from factory i to warehouse j .

$$\text{Minimize } \left(4x_{1,A} + 7x_{1,B} + 7x_{1,C} + x_{1,D} \right) + \left(12x_{2,A} + 3x_{2,B} + 8x_{2,C} + 8x_{2,D} \right) + \left(8x_{3,A} + 10x_{3,B} + 16x_{3,C} + 5x_{3,D} \right)$$

Minimize total shipping cost.

Subject to $x_{1,A} + x_{1,B} + x_{1,C} + x_{1,D} \leq 100$

Supply constraints: $x_{2,A} + x_{2,B} + x_{2,C} + x_{2,D} \leq 200$

$x_{3,A} + x_{3,B} + x_{3,C} + x_{3,D} \leq 150$

$$x_{1,A} + x_{2,A} + x_{3,A} \geq 80$$

Demand constraints: $x_{1,B} + x_{2,B} + x_{3,B} \geq 90$

$$x_{1,C} + x_{2,C} + x_{3,C} \geq 120$$

$$x_{1,D} + x_{2,D} + x_{3,D} \geq 160$$

The Transportation Problem: Matrix Notation

$$\text{Min } \sum_{i=1}^m \sum_{j=1}^n c_{ij} x_{ij}$$

$$\text{s. t. } \sum_{j=1}^n x_{ij} \leq s_i \quad (i = 1, 2, \dots, m) \quad \text{(supply constraints)}$$

$$\sum_{i=1}^m x_{ij} \geq d_j \quad (j = 1, 2, \dots, n) \quad \text{(demand constraints)}$$

$$x_{ij} \geq 0 \quad (i = 1, 2, \dots, m; j = 1, 2, \dots, n)$$

Integer Programming: The Knapsack Problem

How will you select a set of items to put in your backpack so that you can maximize the value of items selected, while respecting a constraint on maximum carrying capacity by you.

$$\text{Let } x_i = \begin{cases} 1 & \text{if item } i \text{ is selected} \\ 0 & \text{otherwise} \end{cases}$$

$$\max \quad \sum_i x_i v_i$$

$$\text{s.t.} \quad \sum_i x_i w_i \leq Q$$

$$x_i \in \{0,1\}$$

- There are m items available.
- Item i weights w_i kg,
- Item i has value v_i .
- You can carry only Q kg.

Optimization of Fed-Batch Bioreactor

Model:

$$\frac{dC_S}{dt} = -\sigma C_X + \frac{u}{V}(C_{S,in} - C_S)$$

$$\frac{dC_X}{dt} = \mu C_X - \frac{u}{V}C_X$$

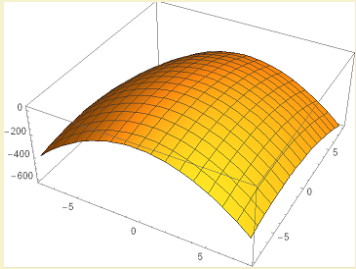
$$\frac{dV}{dt} = u$$

$$\mu = \mu_m \frac{C_S}{K_p + C_S + C_S^2/K_i}$$

$$\sigma = \frac{1}{Y_{X/S}}\mu + m$$

Optimization in Chemical Engineering

Thank You





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

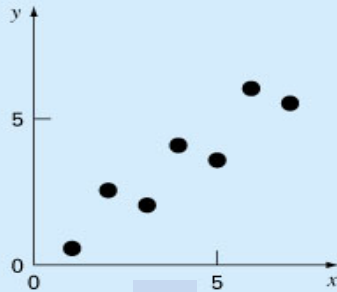
The general problem statement:

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

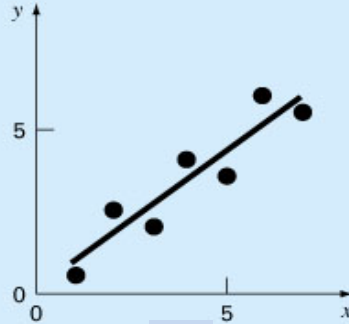
Optimization Problem Formulation: Least Square Regression

Consider Two Cases:

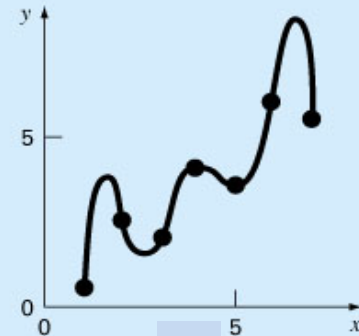
1. Experimental data may exhibit a significant degree of scatter. How to derive a single curve (or line) that represents the general trend of the data?
2. Experimental data may be very precise. How to pass a curve or a series of curves through each of the points?



A



B



C

Least Square Regression: Linear Regression

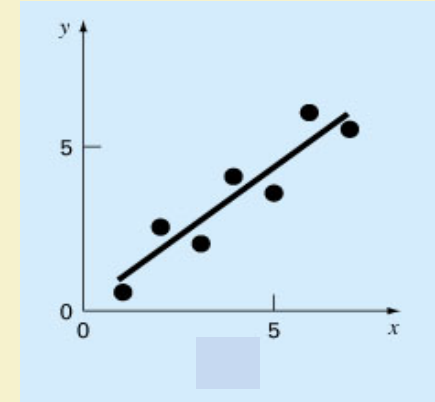
Let us fit a straight line to a set of paired observations: $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$.

$$y = a_0 + a_1 x + e$$

a_1 - slope

a_0 - intercept

e - error, or residual, between the model and the observations



Optimization Problem:

How to find a_0 and a_1 so that the error would be minimum?

Least Square Regression: Linear Regression

Optimization criterion: Minimize the error (residual): $\min \sum_{i=1}^n e_i = \sum_{i=1}^n (y_i - a_0 - a_1 x_i)$

Better optimization criterion: Minimize the square of error (residual):

$$S_r = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i, \text{measured} - y_i, \text{model})^2 = \sum_{i=1}^n (y_i - a_0 - a_1 x_i)^2$$

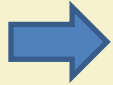
$$\text{Min}_{a_0, a_1} S_r = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - a_0 - a_1 x_i)^2$$

Least Square Regression: Linear Regression

$$\min S_r = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - a_0 - a_1 x_i)^2$$

The coefficients a_0 and a_1 that minimize S_r must satisfy the following conditions:

$$\begin{cases} \frac{\partial S_r}{\partial a_0} = 0 \\ \frac{\partial S_r}{\partial a_1} = 0 \end{cases}$$



$$\begin{aligned} \frac{\partial S_r}{\partial a_0} &= -2 \sum (y_i - a_0 - a_1 x_i) = 0 \\ \frac{\partial S_r}{\partial a_1} &= -2 \sum [(y_i - a_0 - a_1 x_i) x_i] = 0 \\ 0 &= \sum y_i - \sum a_0 - \sum a_1 x_i \\ 0 &= \sum y_i x_i - \sum a_0 x_i - \sum a_1 x_i^2 \end{aligned}$$



$$\begin{aligned} \sum a_0 &= n a_0 \\ n a_0 + \left(\sum x_i \right) a_1 &= \sum y_i \\ \sum y_i x_i &= \sum a_0 x_i + \sum a_1 x_i^2 \end{aligned}$$

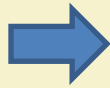
2 equations with 2 unknowns, can be solved simultaneously

Least Square Regression: Linear Regression

$$\sum a_0 = na_0$$

$$na_0 + \left(\sum x_i\right)a_1 = \sum y_i$$

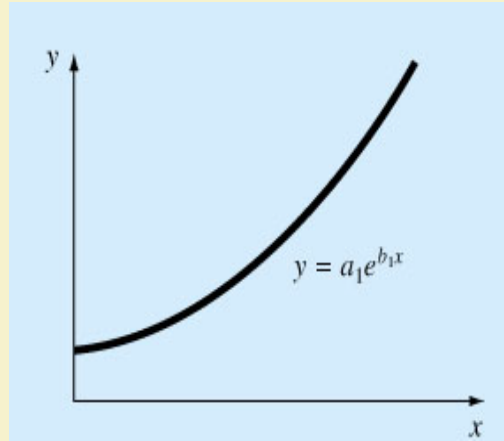
$$\sum y_i x_i = \sum a_0 x_i + \sum a_1 x_i^2$$



$$a_1 = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - (\sum x_i)^2}$$

$$a_0 = \bar{y} - a_1 \bar{x}$$

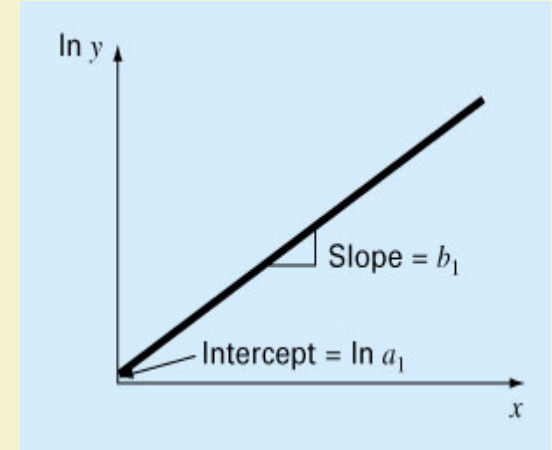
Linearization of Nonlinear Relationship



The exponential equation

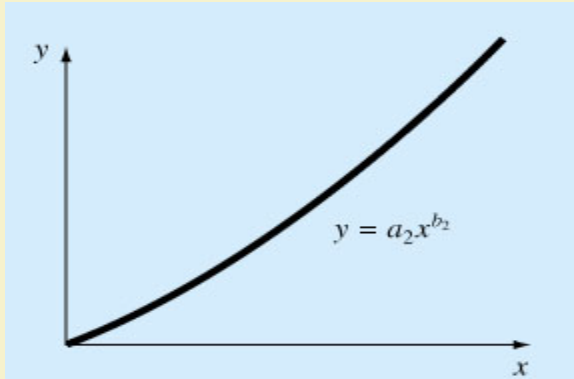
$$\ln y = \ln a_1 + b_1 x$$

$$y^* = a_o + a_1 x$$

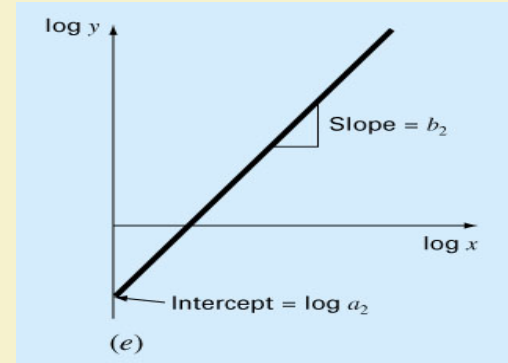


Linearization of Nonlinear Relationship

The power equation



$$\log y = \log a_2 + b_2 \log x$$



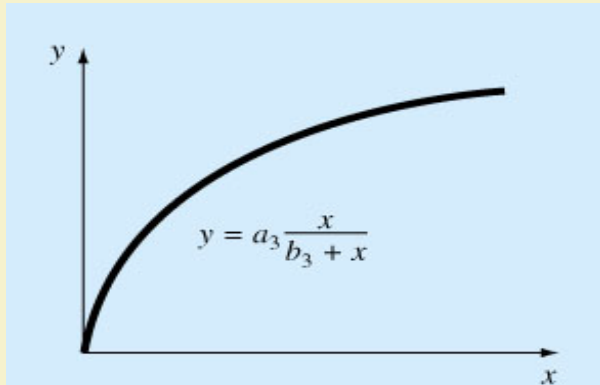
$$\log y = \log a_2 + b_2 \log x$$

Diagram illustrating the linearization of the power equation. The terms $\log y$, $\log a_2$, b_2 , and $\log x$ are circled in purple. Arrows point from these terms to the corresponding terms in the linearized equation below:

$$y^* = a_0 + a_1 x^*$$

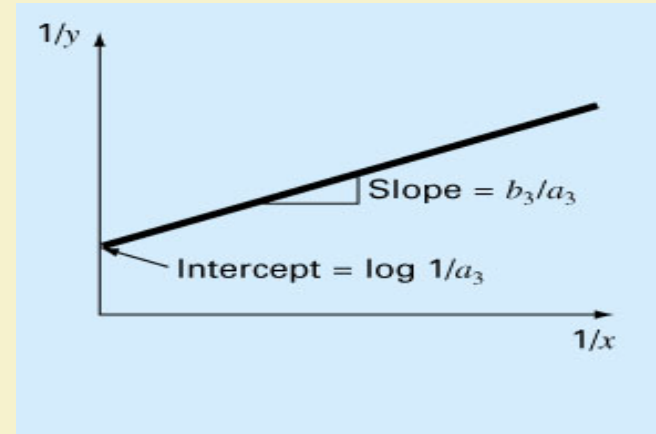
Linearization of Nonlinear Relationships

The saturation-growth-rate equation



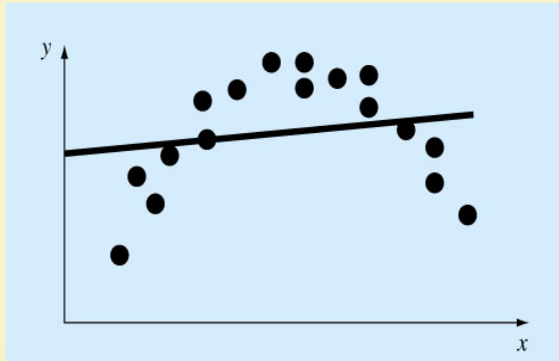
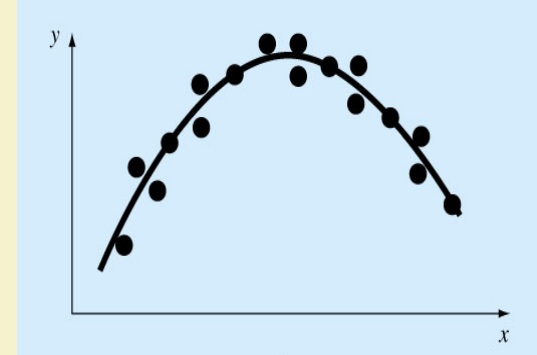
$$\frac{1}{y} = \frac{1}{a_3} + \frac{b_3}{a_3} \left(\frac{1}{x} \right)$$

$$\begin{aligned} y^* &= 1/y \\ a_0 &= 1/a_3 \\ a_1 &= b_3/a_3 \\ x^* &= 1/x \end{aligned}$$



Polynomial Regression

- Not all engineering data can be represented by a straight line.
- For these cases, a curve may be better suited to fit the data.
- The least squares method can readily be extended to fit the data to quadratic or higher order polynomials.



Polynomial Regression

A second order polynomial (quadratic) is defined by:

$$y = a_o + a_1x + a_2x^2 + e$$

The residuals between the model and the data:

$$e_i = y_i - a_o - a_1x_i - a_2x_i^2$$

The sum of squares of the residual:

$$S_r = \sum e_i^2 = \sum \left(y_i - a_o - a_1x_i - a_2x_i^2 \right)^2$$

Polynomial Regression

$$\frac{\partial S_r}{\partial a_o} = -2 \sum (y_i - a_o - a_1 x_i - a_2 x_i^2) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum (y_i - a_o - a_1 x_i - a_2 x_i^2) x_i = 0$$

$$\frac{\partial S_r}{\partial a_2} = -2 \sum (y_i - a_o - a_1 x_i - a_2 x_i^2) x_i^2 = 0$$

$$\sum y_i = n \cdot a_o + a_1 \sum x_i + a_2 \sum x_i^2$$

$$\sum x_i y_i = a_o \sum x_i + a_1 \sum x_i^2 + a_2 \sum x_i^3$$

$$\sum x_i^2 y_i = a_o \sum x_i^2 + a_1 \sum x_i^3 + a_2 \sum x_i^4$$

We have 3 linear equations with 3 unknowns (a_o, a_1, a_2). It can be solved easily.

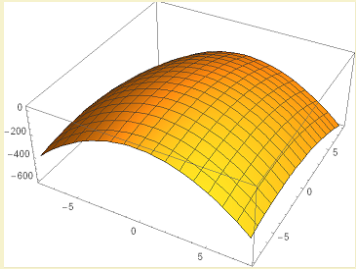
Polynomial Regression: Matrix Notation

A system of 3x3 equations needs to be solved to determine the coefficients of the polynomial.

$$\begin{bmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} \sum y_i \\ \sum x_i y_i \\ \sum x_i^2 y_i \end{Bmatrix}$$

Optimization in Chemical Engineering

Thank You





IIT KHARAGPUR



NPTEL ONLINE
CERTIFICATION COURSES

OPTIMIZATION IN CHEMICAL ENGINEERING

Optimization Problem Formulation

(WEEK – 2: LECTURE – 10)

Dr. Debasis Sarkar

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

Optimization Problem Formulation

Week 2:

-  ☐ Models for optimization
-  ☐ Degrees of freedom analysis
- ☐ Optimization problems in chemical/biochemical engineering

General Problem Formulation

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:

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

Refinery Blending Problem

		Octane	Cost (\$/b)	Available daily
Raw crude oil	1	86	17.00	20,000
	2	88	18.00	15,000
	3	92	20.50	15,000
	4	96	23.00	10,000
		Octane	Price (\$/b)	Maximum daily demand
Petrol	Regular	89	19.50	35,000
	Premium	93	22.00	23,000

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

Let x_{ij} = Number of barrels of raw crude oil of type i ($i = 1, 2, 3, 4$) used per day to make type j ($j = R, P$) petrol

Refinery Blending Problem

		Octane	Cost (\$/b)	Available daily
Raw crude oil	1	86	17.00	20,000
	2	88	18.00	15,000
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	4	96	23.00	10,000
		Octane	Price (\$/b)	Maximum daily demand
Petrol	Regular	89	19.50	35,000
	Premium	93	22.00	23,000

Let x_{ij} = Number of barrels of raw crude oil of type i ($i = 1, 2, 3, 4$) used per day to make type j ($j = R, P$) petrol

Crude oil blended for Regular petrol: $x_{1R} + x_{2R} + x_{3R} + x_{4R}$

Crude oil blended for Premium petrol: $x_{1P} + x_{2P} + x_{3P} + x_{4P}$

Objective function:

$$\text{Maximize } z = 2.5x_{1R} + 1.5x_{2R} - x_{3R} - 3.5x_{4R} + 5.0x_{1P} + 4.0x_{2P} + 1.5x_{3P} - x_{4P}$$

Refinery Blending Problem

		Octane	Cost (\$/b)	Available daily
Raw crude oil	1	86	17.00	20,000
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		Octane	Price (\$/b)	Maximum daily demand
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	Premium	93	22.00	23,000

Let x_{ij} = Number of barrels of raw crude oil of type i ($i = 1, 2, 3, 4$) used per day to make type j ($j = R, P$) petrol

Availability constraints:

$$x_{1R} + x_{1P} \leq 20,000$$

$$x_{2R} + x_{2P} \leq 15,000$$

$$x_{3R} + x_{3P} \leq 15,000$$

$$x_{4R} + x_{4P} \leq 10,000$$

Refinery Blending Problem

		Octane	Cost (\$/b)	Available daily
Raw crude oil	1	86	17.00	20,000
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Let x_{ij} = Number of barrels of raw crude oil of type i ($i = 1, 2, 3, 4$) used per day to make type j ($j = R, P$) petrol

Demand constraint:

$$x_{1R} + x_{2R} + x_{3R} + x_{4R} \leq 35,000$$

$$x_{1P} + x_{2P} + x_{3P} + x_{4P} \leq 23,000$$

Refinery Blending Problem

		Octane	Cost (\$/b)	Available daily
Raw crude oil	1	86	17.00	20,000
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	Premium	93	22.00	23,000

Let x_{ij} = Number of barrels of raw crude oil of type i ($i = 1, 2, 3, 4$) used per day to make type j ($j = R, P$) petrol

Constraint on Octane: $(86x_{1R} + 88x_{2R} + 92x_{3R} + 96x_{4R}) / (x_{1R} + x_{2R} + x_{3R} + x_{4R}) \geq 89$

$$(86x_{1P} + 88x_{2P} + 92x_{3P} + 96x_{4P}) / (x_{1P} + x_{2P} + x_{3P} + x_{4P}) \geq 93$$

Refinery Blending Problem

Constraint on Octane: $(86x_{1R} + 88x_{2R} + 92x_{3R} + 96x_{4R}) / (x_{1R} + x_{2R} + x_{3R} + x_{4R}) \geq 89$

$$(86x_{1P} + 88x_{2P} + 92x_{3P} + 96x_{4P}) / (x_{1P} + x_{2P} + x_{3P} + x_{4P}) \geq 93$$



$$-3x_{1R} - x_{2R} + x_{3R} + 7x_{4R} \geq 0$$

$$-7x_{1R} - 5x_{2R} - x_{3R} + 3x_{4R} \geq 0$$

Refinery Blending Problem

$$\text{Maximize } z = 2.5x_{1R} + 1.5x_{2R} - x_{3R} - 3.5x_{4R} + 5.0x_{1P} + 4.0x_{2P} + 1.5x_{3P} - x_{4P}$$

Subject to:

$$x_{1R} + x_{1P} \leq 20,000$$

$$x_{2R} + x_{2P} \leq 15,000$$

$$x_{3R} + x_{3P} \leq 15,000$$

$$x_{4R} + x_{4P} \leq 10,000$$

$$-3x_{1R} - x_{2R} + x_{3R} + 7x_{4R} \geq 0$$

$$-7x_{1R} - 5x_{2R} - x_{3R} + 3x_{4R} \geq 0$$

$$x_{1R} + x_{2R} + x_{3R} + x_{4R} \leq 35,000$$

$$x_{1P} + x_{2P} + x_{3P} + x_{4P} \leq 23,000$$

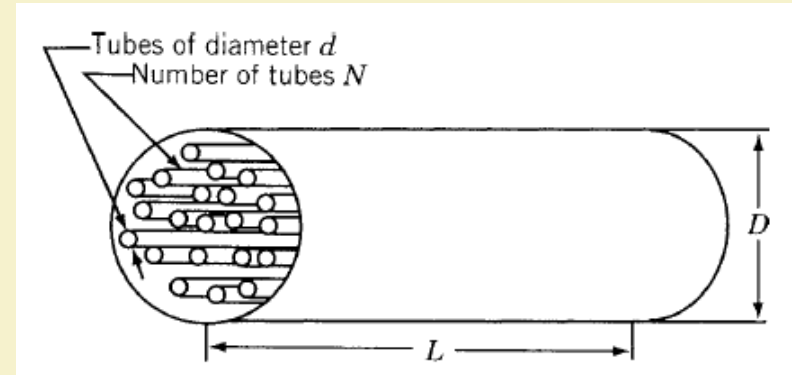
$$x_{1R}, x_{2R}, x_{3R}, x_{4R} \geq 0$$

$$x_{1P}, x_{2P}, x_{3P}, x_{4P} \geq 0$$

Optimization of Shell and Tube Heat Exchanger

- Total length of tubes is equal to at least W_1
- Cost of the tube = W_2 per unit length
- Cost of the shell = $W_3 D^{2.5} L$
- Cost of floor space = W_4 per unit area
- Cost of pumping cold fluid = $W_5 L / d^5 N^2$ per day
- Maintenance cost = $W_6 N d L$
- Thermal energy transferred to the cold fluid is given by $W_7 / N^{1.2} d L^{1.4} + W_8 / d^{0.2} L$
- Thermal energy transferred should be greater than a specified amount W_9

Minimize the overall cost of the heat exchanger



- The expected life of the heat exchanger is W_{10} years
- $W_i, i = 1, 2, \dots, 10$, are known constants
- Each tube occupies a cross-sectional square of width and depth equal to d

Optimization of Shell and Tube Heat Exchanger

Decision variables: D , L , d , and N

Objective function:

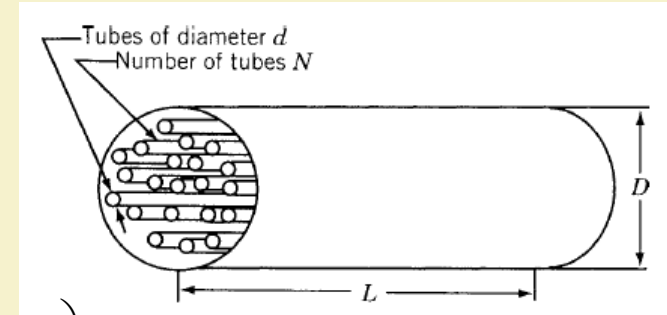
Overall cost = cost of tube + cost of shell + cost of floor space + cost of pumping cold fluid + cost of maintenance

$$\text{Min } f(D, L, d, N) = W_2 NL + W_3 D^{2.5} L + W_4 DL + W_{10} \left(\frac{W_5 L}{d^5 N^2} + W_6 NdL \right)$$

Constraint on total length: $NL \geq W_1$

Constraint on thermal energy transferred: $\frac{W_7}{N^{1.2} d L^{1.4}} + \frac{W_8}{d^{0.2} L} \geq W_9$

Constraint on cross-sectional area: $\frac{\pi D^2}{4} \geq Nd^2$



Non-negativity constraint:

$$D \geq 0, L \geq 0, d \geq 0, N \geq 0$$

Net Present Value

One approach to evaluate the economics of a project/decision is to use Net Present Value (NPV). Here we convert all economic transactions to equivalent values in the present.

In general, outflows (expenses) are considered negative; inflows (savings or income) are considered positive.

The present value, P , of one future payment or receipt, F , at period n with interest rate i is:

$$P = \frac{F_n}{(1+i)^n}$$

The present value of a series of uniform payments, A , where the first payment is made at the end of the first period is given by:

$$P = A \frac{(1+i)^n - 1}{i(1+i)^n}$$

Net Present Value: An Example

We can buy a heat pump for INR 50,000 which will work for 5 years. The pump can save INR 12,000 per year. If an interest rate of 10% is assumed, is the heat pump a good investment?

Solution:

The initial expense of the pump, INR 50,000, is already in the present, so this does not need to be converted. We will consider it negative since it is money paid out (expense).

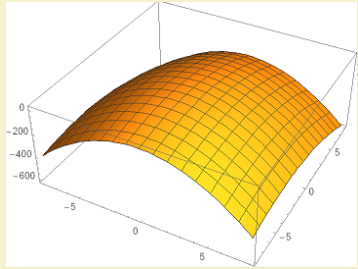
The present value of the savings is given by,

$$P = 12000 \frac{(1+0.1)^5 - 1}{0.1(1+0.1)^5} = 45489$$

Since the Net Present Value is negative, this is not a good investment.

$$NPV = -50000 + 45489 = -4510$$

Optimization in Chemical Engineering



Thank You
End of Week 2

