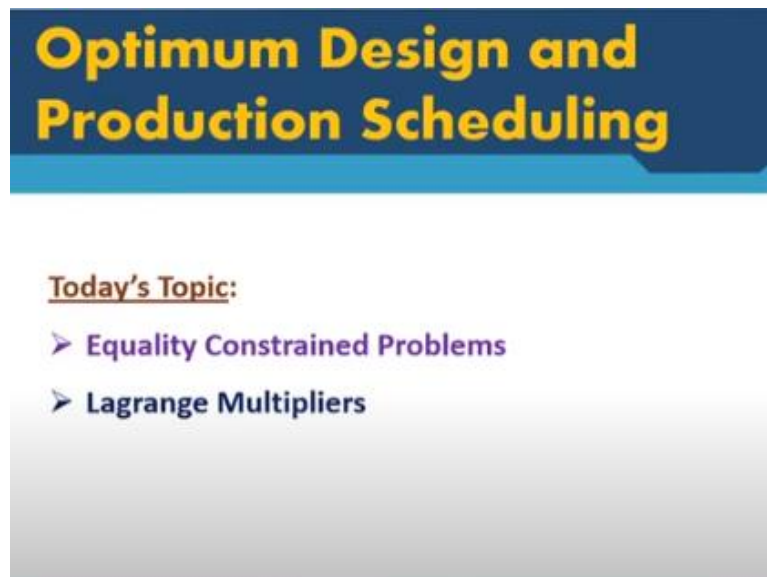


Plant Design and Economics
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Lecture - 58
Equality Constrained Problems: Lagrange Multipliers

Welcome to lecture 58 of Plant Design and Economics. In this module as of now we have talked about optimality criteria for unconstrained single variable and multivariable functions. We have also seen several examples on applications of these optimality criterion. Now today we will talk about the optimization problems with equality constraints. So we will talk about the optimality criteria for equality constrained optimization problems.

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**Optimum Design and
Production Scheduling**

Today's Topic:

- Equality Constrained Problems
- Lagrange Multipliers

And the method for solutions of such equality constrained problems by Lagrange multipliers technique.

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Unconstrained Vs Constrained Functions

Unconstrained optimization finds a 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.

Example: Catalyst deactivation puts upper limit on temperature, Product specification must be met, Mass balances must be met, etc.

Unconstrained Optimization:

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

Answer: 4

Constrained Optimization:

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

Answer: 5

When you solve an unconstrained optimization problem, we assume that the decision variable can take on any possible value. But, this will in general be not possible because the additional constraints exist that limit the range of feasible values for decision variables. Suppose, you are designing a chemical reactor. So let us say to increase the rate of the reaction you would like to operate the reactor at high temperature.

But you are not free to take a temperature as high as you want because there may be operational constraint imposed on the process. If it is a catalyzed reactor, the catalyst may get deactivated. So a restriction or constraint will be imposed on the temperature. A product specification must be made. So constraints on the product specifications will be imposed.

Similarly, while solving an optimization problem related to a process, the mass balances must be respected. These mass balances will come as equality constraints. So in actual practice we will have constrained optimization problems. The solutions of constrained optimization problem will of course be different from solution so unconstrained optimization problem.

For example, let us take this simple example $f(x) = (x-4)^2$. Now when the function is unconstrained, or the decision variables can take on any values, obviously the answer is $x = 4$. Because then at that case, the $f(x)$ takes value equal to zero. And

since $f(x)$ is a square of a term, it cannot be less than zero. So $x = 4$ is the minimum of $f(x) = (x - 4)^2$.

Let us now put a constraint to the same objective function $f(x) = (x - 4)^2$ and I say x now can take on values which are greater or equal to 5. So obviously, now the answer is $x = 5$. Any value greater than 5 will make $f(x)$ value higher and we are minimizing the function. So when I say $x = 5$, the function value is 1. When I take $x = 6$, the function value is $6 - 4 = 2$ square equal to 4.

But I can now take $x = 4$ because x has to be greater or equal to 5. So the minimum value for this constrained function now is $x = 5$.

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Equality Constrained Functions: Variable Elimination Method

Minimize $f(x)$
 Subject to: $h_i(x) = 0 \quad \forall i = 1, \dots, m$
 $x \in \mathbb{R}^n$

Example: ✓
 Min $f(x) = 4x_1^2 + 5x_2^2$
 Subject to: $2x_1 + 3x_2 = 6$

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

Min $f(x_2) = (6 - 3x_2)^2 + 5x_2^2 + 10$

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.

Let us consider this constrained optimization problem and we are talking only equality constrained optimization problem. That means the constraints are equality type. So we have only one type of constraints, all the constraints are equality type. There may be any number of such constraints, but inequality type constraints are not present, only equality type constraints are present.

So we are minimizing this function $f(x)$ subject to m number of constraints. So which can be written as $h_i(x) = 0$. So $h_1 = 0, h_2 = 0$ up to $h_n = 0$. And x takes values in the real space. So now the optimization problem is a constrained problem, number one. And the minimization of $f(x)$ will be satisfied by these constraints. So the

values of x that minimize $f(x)$ must satisfy the constraints $h_i(x) = 0$ for all the constraints.

So $h_1(x) = 0, h_2(x) = 0$ up to $h_m(x) = 0$. Now an equality constrained optimization problem, you can in principle solve by converting to an equivalent unconstrained problem. So how do you do that? If it is possible to explicitly eliminate these variables, the decision variables using the equality constraints, then it is possible. For example, let us consider this case.

I have an equality constrained optimization problem $f(x) = 4x_1^2 + 5x_2^2$ subject to $2x_1 + 3x_2 = 6$. What I say that an equality constrained optimization problem can be solved by converting it to an unconstrained problem by explicitly eliminating m independent variables using the m equality constraints. So now we make use of this constraint $2x_1 + 3x_2 = 6$ to replace one of this decision variables x_1 or x_2 .

Then it will be a decision variable or single variable. Then it will be an objective function of single decision variable. And also it will be unconstrained in nature. So let us say from this $2x_1 + 3x_2 = 6$ we can obtain $x_1 = \frac{6 - 3x_2}{2}$. So now I can rewrite my original objective function as a function of x_2 alone. And this becomes an unconstrained function.

Note that these constraint has now been incorporated in the objective function itself. You are still solving an unconstrained optimization problem by solving sorry you are still solving a constrained optimization problem by solving an unconstrained optimization problem. You basically have incorporated the constraint into the objective function.

Now it may not always be possible to explicitly eliminate these decision variables one by one. And if you have m number of decision variables, it may not be possible to eliminate you know each of these $m - 1$ decision variables using those equality constraints and express the objective function as a function of single decision variable.

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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)



So we have this method of Lagrange multipliers for solutions of such equality constrained optimization problem. But for simple problems of course, you can make use of this variable elimination method to convert the equality constrained optimization problem to an equivalent unconstrained optimization problem.

The method of Lagrange multipliers gives a set of necessary conditions for candidate optimal solutions of equality constrained optimization problem. In this method, an equality constrained problem is converted to an equivalent unconstrained problem with help of certain unspecified parameters which we call Lagrange multipliers. So we will introduce Lagrange multipliers which are unspecified parameters.

And with help of those, we convert the equality constrained optimization problem to an equivalent unconstrained optimization problem. How do I do that? Suppose, I have an objective function and let us say two equality constraints. So I will introduce two Lagrange multipliers. So I will introduce one Lagrange multiplier for each equality constraint. Then, formulate an unconstrained optimization problem as follows.

Take the objective function then add to it a product of Lagrange multiplier and the corresponding equality constraint. So if I have two constraints say $h_1 = 0$, $h_2 = 0$. So both are functions of the decision variables. So and $f(x)$ is my objective function. So I can convert these constrained optimization problem to an equivalent unconstrained optimization problem by formulating an unconstrained objective function as $f(x) + \lambda_1 h_1 + \lambda_2 h_2$.

This we call as Lagrangian. Let us we look at this in the next slides. So each equality constraint is associated with a Lagrange multiplier. Their values depend on the form and the form of the objective function as well as on the form of the constrained functions. If the functional form of the constraint changes the value of the Lagrange multiplier also changes. So remember that for each equality constraint we will associate one Lagrange multiplier.

And the values of this Lagrange multiplier depend on the form or the functional form of the objective function and the constrained functions.

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Method of Lagrange Multipliers: A Single Equality Constraint

Consider:

$$\begin{aligned} & \text{Min}_{x_1, x_2} f(x_1, x_2) \\ & \text{s.t. } h(x_1, x_2) = 0 \end{aligned}$$

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 x^* and x^* also satisfies $h(x^*)=0$, then x^* minimize the original constrained problem: $\text{Min } L(x^*, \lambda^*) = \text{Min } f(x)$

Let us look at this equality constrained optimization problem. We have an objective function of two variables and we have a single equality constraint which is of course a function of these two decision variables. So what will be my Lagrangian? So what is Lagrangian? The method of Lagrange multipliers converts this constrained problem to an equivalent unconstrained problem. How?

We consider one Lagrange multiplier for each constraint. I have one constraint here. So I assume only one Lagrange multiplier, let us say lambda. So I formulate the unconstrained optimization problem as $f(x)$. So this is f of x_1 and x_2 plus lambda into h . So this new function which is a now function of the original decision variables as well as the unspecified parameter that we have introduced Lagrange multiplier lambda.

So this function let us call L is a function of x_1 , x_2 and λ . We call this function as Lagrangian function. So the first step towards solving equality constrained problems using Lagrange multipliers is to formulate this Lagrangian. So how will you formulate the Lagrangian? You will specify one Lagrange multiplier for each equality constraint. Then, multiply the equality constraint with its corresponding Lagrange multiplier.

Then add this with the objective function. Repeat for each equality constraint you have. So then you obtain a function like this, which we will call as Lagrangian. So L is the Lagrangian and λ is the Lagrange multiplier. Note that the Lagrange multiplier is unspecified parameter. So the value of the Lagrangian multiplier will also be determined optimally along with the value of x_1 and x_2 .

So once you have this unconstrained function now I can apply whatever I have learned as optimality criteria for unconstrained problems. So it will always be multivariable problems. So whatever we have learned as optimality criteria for unconstrained multivariable functions now I can apply those criteria on this which is an unconstrained function, the Lagrangian is an unconstrained function.

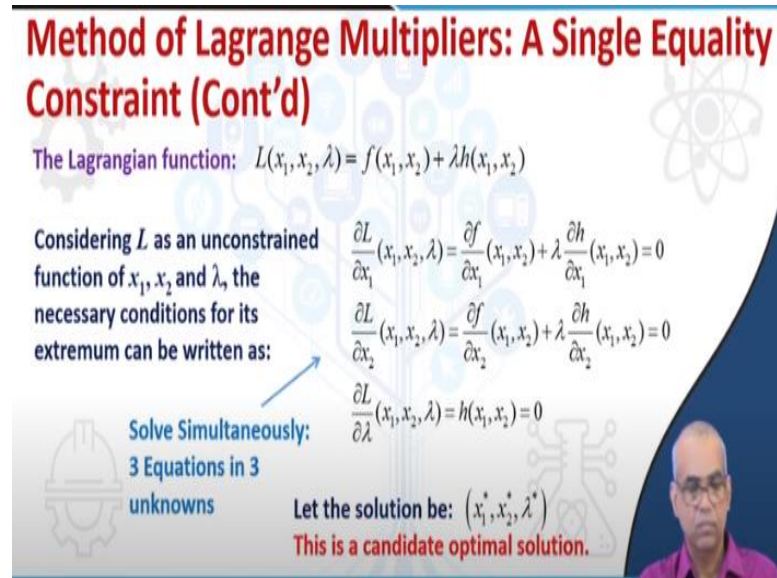
So I will apply the optimality criteria for unconstrained multivariable functions to this Lagrangian. And that way thereby I will solve the equality constrained optimization problem. Note that there is no sign restriction on this Lagrange multiplier. So Lagrange multiplier can take values with any sign. Now this is my Lagrange multiplier. This is my Lagrangian in which the constraints have been incorporated.

Now let us apply the optimality conditions for multivariable functions to these Lagrangian. Now if the solution that I get, that means let us say I am minimizing this problem. So the solution that means x_1 , x_2 and λ that minimizes these Lagrangian function also satisfies this constraint then the solution for this Lagrangian and the solutions for this original problem is same. I repeat this.

I want to minimize this problem which is an equality constrained problem. I formulate this Lagrangian. Now let us consider that I have obtained the minimum point for this

Lagrangian. Let us consider that as x_1^* , x_2^* and λ^* . So x_1^* , x_2^* and λ^* minimizes this Lagrangian function. Now if that x_1^* , x_2^* also satisfies these equality constraint then the x_1^* and x_2^* also solves this optimization problem. So this is the principle of Lagrange multiplier techniques.

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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:
3 Equations in 3 unknowns

Let the solution be: $(x_1^*, x_2^*, \lambda^*)$
This is a candidate optimal solution.

So now obtaining the optimality criteria will be straightforward because we will straightaway apply the optimality conditions for unconstrained multivariable function. So what we do is we set $\frac{\partial L}{\partial x_1}$ equal to zero. Set $\frac{\partial L}{\partial x_2}$ equal to zero. And set $\frac{\partial L}{\partial \lambda}$ equal to zero. Note that in the Lagrangian all x_1 , x_2 and λ are now variables.

λ is the unspecified parameter whose value also has to be found out optimally along with x_1 and x_2 . So Lagrangian is a function of x_1 , x_2 and λ . So the optimality criteria for unconstrained optimization problems will require you to set $\frac{\partial L}{\partial x_1}$, $\frac{\partial L}{\partial x_2}$ equal to zero. Gradient of the Lagrangian equal to zero. So that will be $\frac{\partial L}{\partial x_1}$ equal to zero, $\frac{\partial L}{\partial x_2}$ equal to zero and $\frac{\partial L}{\partial \lambda}$ equal to zero.


So these three conditions will give you three equations and three variables x_1 , x_2 and λ . So you can solve simultaneously. If the solution is x_1^* , x_2^* and λ^* so then this becomes a candidate optimal solution.

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Method of Lagrange Multipliers: General Problem

Consider: Minimize $f(x)$ $x = n$ -vector ✓
 subject to $h_j(x) = 0, j = 1, 2, \dots, m$ ✓

$\lambda_1, \lambda_2, \dots, \lambda_m$

$$L = f(x) + \lambda_1 h_1 + \lambda_2 h_2 + \dots + \lambda_m h_m$$


Now we saw the examples with one equality constraint. You can just extend it you can extend it to any number of equality constraint. Let us consider I have a function, objective function in n variables and I have m number of equality constraints. So how do I formulate the Lagrangian? So for m equality constraints I define m Lagrangian multipliers; λ_1, λ_2 up to λ_m .

Then take λ_1 into h_1 plus λ_2 into h_2 up to λ_m into h_m and also add the function, objective function $f(x)$. So that gives me the Lagrangian.

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Method of Lagrange Multipliers: General Problem

Consider: Minimize $f(x)$ $x = n$ -vector ✓ n
 subject to $h_j(x) = 0, j = 1, 2, \dots, m$ ✓

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

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


The necessary conditions are given as:

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

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

Eq.: $(n + m)$, Unknowns: $(n + m)$
 Solve simultaneously.

$n + m$ Eq
 $n + m$ Variable



So this is how we will do for the general problems where objective function has n variables and you have m number of equality constraints. So this can be written more compactly using the summation notation. So the necessary conditions will be obtained

as taking the derivatives of this Lagrangian and function with respect to each decision variables and each Lagrange multipliers.

So there are n variables and m number of equality constraints. So you will have $\frac{\partial L}{\partial x_i}$ where i equal to 1 to n equal to zero and then $\frac{\partial L}{\partial \lambda_j}$ where j equal to 1 to m for the Lagrange multipliers. So note that this will give you $n + m$ number of equations. So you have n number of decision variables. So $\frac{\partial L}{\partial x_1}$, $\frac{\partial L}{\partial x_2}$, $\frac{\partial L}{\partial x_3}$ up to $\frac{\partial L}{\partial x_n}$ equal to zero. That gives me n number of equations.

And you have m number of equality constraints. So m number of Lagrange multipliers. So you said $\frac{\partial L}{\partial \lambda_1}$ equal to zero, $\frac{\partial L}{\partial \lambda_2}$ equal to zero up to $\frac{\partial L}{\partial \lambda_m}$ equal to zero. So this gives me m number of equations. So $n + m$ number of total equations I get and my variables are also n number of decision variables and m number of Lagrange multipliers.

So I have $n + m$ equations and $n + m$ variables. So it is possible for me in principle to solve and we can obtain the values of x_1 to x_n as well as λ_1 to λ_m . That minimizes or solves my optimization problem.

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Method of Lagrange Multipliers: General Problem

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

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

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

The necessary conditions are given as:

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

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

Eq.: $(n + m)$, Unknowns: $(n + m)$
Solve simultaneously.

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

fsolve

See note that there may be multiple solutions. Also it may not always be possible to solve these equations by hand. Often times this when you said $\frac{\partial L}{\partial x_i}$ equal to zero, $\frac{\partial L}{\partial \lambda_j}$ equal to zero the equations that you get may be nonlinear in nature and you can make use of any software that solves nonlinear equations for that. For

example, if you have access to MATLAB, you can use `f solve` to solve the resulting nonlinear equations if it happens.

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Lagrange Multipliers: Example-1

A company manufactures two types of fertilizers (A, B) in a plant. The total cost of production, C_T (in INR) depends on amount of each fertilizer produced and is approximated by the function $C_T = 5x^2 + 2xy + 3y^2 + 1500$

Here, x = tons of fertilizer-A produced, y = tons of fertilizer-B produced

If the total amount of fertilizer (both types combined) to be produced per day is 60 tons, find the daily production plan that minimizes the production cost.

Solution:

Problem Formulation:

Minimize $C_T = 5x^2 + 2xy + 3y^2 + 1500$ over x, y

subject to $x + y = 60$

Handwritten notes on the slide include a checkmark next to the cost function, and the constraint equation $x + y - 60 = 0$ written in blue ink.

Now let us take one example. A company manufactures two types of fertilizers A and B in a plant. The total cost of production C_T in Indian rupees depends on amount of each fertilizer produced and is approximated by the function C_T equal to $5x^2$ plus $2xy$ plus $3y^2$ plus 1500. x equal to tons of fertilizer A produced and y equal to tons of fertilizer B produced.

If the total amount of fertilizer both types combined A plus B to be produced per day is 60 tons, find the daily production plan that minimizes the production cost. So how much of fertilizer A and how much of fertilizer B, that means how many tons of fertilizer A and how many tons of fertilizer B we have to produce per day so that we can minimize the daily production cost.

So we will solve this using Lagrange multiplier. So let us formulate the problem first. We minimize this cost function. So I assume that x equal to tons of fertilizer A to be produced and y equal to tons of fertilizer B to be produced per day. So C_T equal to as given and it must satisfy the equality constraint $x + y = 60$ because the daily production must be equal to 60 tons, exactly 60 tons. So $x + y = 60$. You can also write as $x + y - 60 = 0$.

(Refer Slide Time: 27:44)

Lagrange Multipliers: Example-1

Solution (Cont'): Minimize $C_f = 5x^2 + 2xy + 3y^2 + 1500$
subject to $x + y = 60$

$$\begin{aligned} \text{Min } f(x_1, x_2) \\ \text{s.t. } h(x_1, x_2) = 0 \end{aligned}$$

Lagrangian Function: $L = (5x^2 + 2xy + 3y^2 + 1500) + \lambda(x + y - 60)$

Necessary Conditions:

$$\frac{\partial L}{\partial x} = 10x + 2y + \lambda = 0$$

$$\frac{\partial L}{\partial y} = 2x + 6y + \lambda = 0$$

$$\frac{\partial L}{\partial \lambda} = x + y - 60 = 0$$

Solve:

From first two equations: $8x - 4y = 0$

Combine with last equation: $12x - 240 = 0 \Rightarrow x = 20$

Hence, $y = 60 - 20 = 40$

Optimal Production Plan:
20 tons of A and 40 tons of B

So now let us solve it using Lagrange multiplier method. Formulate the Lagrangian function. So introduce one Lagrange multiplier lambda. So the objective function f x or CT here plus lambda into the equality constraint. So the Lagrangian gives me the unconstrained function to be minimized. So set del L del x = 0, set del L del y = 0 and set del L del lambda = 0.

You have three equations and three variables x, y and lambda. All are linear equations, very easy to solve these equations. For example, from the first two equations, if you simply subtract the second equation from the first one, you will obtain $8x - 4y = 0$. Now combine this with the last equation. Combine this with this last equation. Simply multiply by this del $x + y - 60 = 0$ by 4 and then add it up with this.

And you will obtain $12x - 240 = 0$ which gives $x = 20$. So total is 60 tons. So the y will be $60 - 20 = 40$. So 20 tons of fertilizer A, 40 tons of fertilizer B. So that should be my optimal production plan.

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Lagrange Multipliers: Example-2

Minimize $f = x^2 + y^2 + z^2$
 x, y, z

subject to $3x + y + z = 5$

$x + y + z = 1$

Lagrangian Function:

$$L = (x^2 + y^2 + z^2) + \lambda_1(3x + y + z - 5) + \lambda_2(x + y + z - 1)$$

Necessary Conditions:

$$\frac{\partial L}{\partial x} = 2x + 3\lambda_1 + \lambda_2 = 0$$

$$\frac{\partial L}{\partial \lambda_1} = 3x + y + z - 5 = 0$$

$$\frac{\partial L}{\partial y} = 2y + \lambda_1 + \lambda_2 = 0$$

$$\frac{\partial L}{\partial \lambda_2} = x + y + z - 1 = 0$$

$$\frac{\partial L}{\partial z} = 2z + \lambda_1 + \lambda_2 = 0$$

$$\begin{bmatrix} 2 & 0 & 0 & 3 & 1 \\ 0 & 2 & 0 & 1 & 1 \\ 0 & 0 & 2 & 1 & 1 \\ 3 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 5 \\ 1 \end{bmatrix}$$

Another example minimize f equal to x square plus y square plus z square subject to $3x + y + z = 5$, $x + y + z = 1$. I have now two equality constraint. Formulate the Lagrangian. So introduce two Lagrange multipliers lambda 1 and lambda 2. Set the necessary conditions del L del x = 0, del L del y = 0, del L del z = 0. And also del L del lambda 1 equal to 0 and del L del lambda 2 equal to 0.

Now we have five variables x, y, z, lambda 1, lambda 2 and five equations. You can solve it. In fact you can, all are linear equations, so you can write this x equal to b form.

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Lagrange Multipliers: Example-2

$$\begin{bmatrix} 2 & 0 & 0 & 3 & 1 \\ 0 & 2 & 0 & 1 & 1 \\ 0 & 0 & 2 & 1 & 1 \\ 3 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 5 \\ 1 \end{bmatrix}$$

$$AX = b$$

$$\Rightarrow X = A^{-1}b$$

$$\Rightarrow \begin{bmatrix} x \\ y \\ z \\ \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 2 \\ -1/2 \\ -1/2 \\ -5/2 \\ 7/2 \end{bmatrix}$$

And the solution will be x equal to A inverse B. So by matrix inversion method or Kramer's rule, you can obtain this solution. So this is possible only for linear

equations like this. So had it been nonlinear, so it perhaps will be necessary to make use of a software to solve the resulting nonlinear equations.

For large nonlinear large number of nonlinear equations, solutions by hand will be really time consuming and may be difficult and cumbersome.

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Example-3: Optimization of a CSTR

A feed stream carrying only reactant A with concentration C_{A0} mol/m³ enters a CSTR with volumetric feed-rate F m³/h and undergoes a first order reaction $A \rightarrow B$.

The rate of formation of B is given as $r_B = kC_A$ where $k = 0.1 \text{ h}^{-1}$ is the reaction rate constant.

We wish to produce 10 mol/h of B and cost of this operation per hour (C_T Rs/h) can be expressed as sum of two cost components: cost of feed A and cost of utility that depends on CSTR volume (V m³), as follows: $C_T = 5C_{A0}F + 0.3V$

If the initial concentration of A, $C_{A0} = 0.04 \text{ mol/m}^3$, find the minimum cost of operation.

Now let us take one more example, a slightly more involved example. It is about optimization of a CSTR. A feed stream carrying only reactant A with concentration C_{A0} mole per meter cube enters a CSTR with volumetric feed rate F meter cube per hour and it undergoes a first order reaction A to B within the CSTR. The rate of formation of B is given as $r_B = kC_A$ where $k = 0.1 \text{ hour}^{-1}$ is the reaction rate constant.

We used to produce 10 mole per hour of B and the cost of this operation per hour C_T rupees per hour can be expressed as a sum of two cost components, cost of feed A and cost of utility that depends on CSTR volume V as follows $C_T = 5C_{A0}F + 0.3V$. If the initial concentration of A, $C_{A0} = 0.04$ mole per meter cube find the minimum cost of operation.

So to summarize you have a CSTR where a first order reaction is taking place. The rate constrained is given. We want to produce exactly 10 mole per hour of B and the cost of production or cost of this operation is given as a function of C_{A0} feed rate as

well as volume. C_{A0} is specified as 0.04 mole per meter cube, okay? So we have to find the minimum cost of operation. So how do I solve this problem?

So you have to minimize this cost of operation C_T equal to 5 into C_{A0} into f plus 0.3 into V . Note that C_{A0} is specified as 0.04.

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Optimization of a CSTR: How to Solve?

In order to minimize the cost of operation, we need to determine the optimal values of reactor volume (V), feed rate (F), and concentration of A in the reactor (C_A). Formulate a constrained optimization problem to determine optimal V , F and C_A . Use mass balance equations on A and B to formulate these constraints. Use method of Lagrange multipliers to derive the expressions for optimal V , F , and C_A .

Material Balance:
 Accumulation = Input - Output

$FC_B = 10 \text{ mol/h}$
 $\frac{\text{mol}}{\text{h}} = \frac{\text{mol}}{\text{m}^3} \times \frac{\text{m}^3}{\text{h}}$

The diagram shows a CSTR with an inlet stream labeled F, C_{A0} and an outlet stream labeled F, C_A, C_B . Inside the reactor, the reaction is $A \rightarrow B$ and the volume is V . Handwritten notes include the material balance equation and a calculation for the outlet flow rate of B.

Now in order to minimize the cost of operation, we have to determine the optimal values of reactor volume V , the feed rate F and also the concentration of A in the reactor. So concentration of A in the reactor and the concentration of A in the effluent is same. And we have to do this such that the amount of B right, the moles per hour of B in the outlet is exactly 10. So 10 moles per hour of B is obtained.

So F into C_B will be 10 moles per hour. So the concentration within the reactor is same as concentration outside the reactor effluent stream here because of CSTR. So in the objective function there was no C_A or C_B . But note that this will be this has to be taken care of. Because this determines the fact that we have to find out the operating condition such that we have the B as 10 moles per hour.

So F is volumetric feed rate. So that will be like meter cube per hour and C_B the concentration of B will be moles per meter cube. So it will be moles per hour. So F into C_B must be 10 moles per hour.

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Example-3: Optimization of A CSTR: Formulation

Material Balance: Accumulation = Input - Output

Material balance on A

$$0 = C_{A0}F - (r_A V + FC_A)$$

$$\Rightarrow (C_{A0} - C_A)F - 0.1C_A V = 0$$

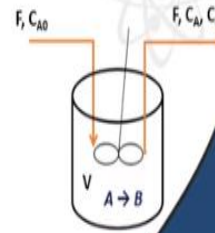
Note: $r_B = kC_A$ where $k = 0.1 \text{ h}^{-1}$

Material balance on B

$$0 = r_B V - FC_B$$

$$\Rightarrow 0.1C_A V - 10 = 0$$

(Because we want to produce 10 mol/h of B)



Optimization Problem Formulation:

Minimize $C_T = 5C_{A0}F + 0.3V$

Subject to $(C_{A0} - C_A)F - 0.1C_A V = 0$

$0.1C_A V - 10 = 0$

So to obtain those constraints, we have to write down the material balance on A and material balance on B. So what is the mass balance on A? The A enters with the feed stream. How much? C_{A0} into F moles per hour because F is meter cube per hour and C_{A0} in mole per meter cube. So this amount enters to the reactor and what goes out is F into C_A and also it gets consumed. It is converted to, it gets reacted to B.

So r_A into V . So r_A is 0.1 into C_A . So after putting these values you can obtain this. So this is one constraint that I obtained from material balance on A. This must be respected. Similarly, we can we have to also write material balance on B. There is no B entering, but B leaving as F into C_B and B is being formed due to reaction within the reactor that is r_B into V . So that is 0.1 into C_A into V .

And then FC_B is 10 because we want to produce 10 mole per hour of B. So this is another equality constraint. So this is one equality constraint and this is another equality constraint. So now I am in a position to write down the problem. So I formulate the optimization problem as follows. Minimize C_T equal to F into $C_{A0}F$ plus 0.3 into V as given.

But then I have these two equality constraints. One from material balance on A, another from material balance on B.

(Refer Slide Time: 37:24)

Example-3: Optimization of A CSTR

The Lagrangian Function:

$$L = [5C_{A0}F + 0.3V] + \lambda_1 [(C_{A0} - C_A)F - 0.1C_A V] + \lambda_2 [0.1C_A V - 10]$$

$$\left\{ \begin{array}{l} \frac{\partial L}{\partial F} = 5C_{A0} + \lambda_1(C_{A0} - C_A) = 0 \\ \frac{\partial L}{\partial V} = 0.3 - 0.1\lambda_1 C_A + 0.1\lambda_2 C_A = 0 \\ \frac{\partial L}{\partial C_A} = -\lambda_1 F - 0.1\lambda_1 V + 0.1\lambda_2 V = 0 \end{array} \right. \quad \left\{ \begin{array}{l} \frac{\partial L}{\partial \lambda_1} = (C_{A0} - C_A)F - 0.1C_A V = 0 \\ \frac{\partial L}{\partial \lambda_2} = 0.1C_A V - 10 = 0 \end{array} \right.$$

So make use of Lagrange multipliers method. We have two equality constraint introduced to Lagrange multipliers, lambda 1 and lambda 2. Formulate the Lagrangian function. So you have now five variables actually. Three variables as flow rate feed flow rate, volume of the reactor, and concentration of A within the reactor and the other two are Lagrange multipliers lambda 1 and lambda 2.

So set del L del F = 0, del L del V = 0, del L del C A = 0. Del L del lambda 1 = 0, del L del lambda 2 = 0. Five variables five equations you will be able to solve.

(Refer Slide Time: 38:14)

Example-3: Optimization of A CSTR

The Lagrangian Function: $L = [5C_{A0}F + 0.3V] + \lambda_1 [(C_{A0} - C_A)F - 0.1C_A V] + \lambda_2 [0.1C_A V - 10]$

$$\left\{ \begin{array}{l} \frac{\partial L}{\partial F} = 5C_{A0} + \lambda_1(C_{A0} - C_A) = 0 \\ \frac{\partial L}{\partial V} = 0.3 - 0.1\lambda_1 C_A + 0.1\lambda_2 C_A = 0 \\ \frac{\partial L}{\partial C_A} = -\lambda_1 F - 0.1\lambda_1 V + 0.1\lambda_2 V = 0 \\ \frac{\partial L}{\partial \lambda_1} = (C_{A0} - C_A)F - 0.1C_A V = 0 \\ \frac{\partial L}{\partial \lambda_2} = 0.1C_A V - 10 = 0 \end{array} \right.$$

Solve simultaneously

F	12182 m ³ /h
V	31455 m ³
C _A	0.0318 mol/m ³

$$C_T = 5C_{A0}F + 0.3V = 11872.9 \text{ Rs/h}$$

So you have to solve these equations simultaneously. Here MATLAB's Fsolve was used for this and we obtain the solutions as F = 12182 meter cube per hour. V = 31455 meter cube and C A = 0.0318 mole per meter cube. So these are the optimal

values of feed flow rate, volume of the CSTR and the concentration of A in the reactor which minimizes the cost of operation given as $C_T = 5C_{A0}F + 0.3V$.

Putting all the values and putting the values of C_{A0} as given we obtain the minimum cost as 11872.9 Rs/h. With this we will stop our discussion here.