

**Optimization in Chemical Engineering**  
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**Lecture - 60**  
**Software Tools for Optimization (Contd.)**

Welcome to lecture 60. So, this is the last lecture for this course. As of now we have talked about Optimization problems where the decision variable to continuous values, but you will encounter several Optimization problems where the decision variables or at least some of the decision variables can take integer values like 0 1 2 3 etcetera.

In some problems the decision variables can take only 0 or 1 values. So, in this lecture I will try to briefly introduce such integer programming problems.

So, we will take a very simple example and talk about a method known as branch and bound method to explain how such problems can be solved using branch and bound method, but it will be at a very introductory level.

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**Software Tools for Optimization**

Week 12:

- MATLAB, EXCEL Solver for Optimization

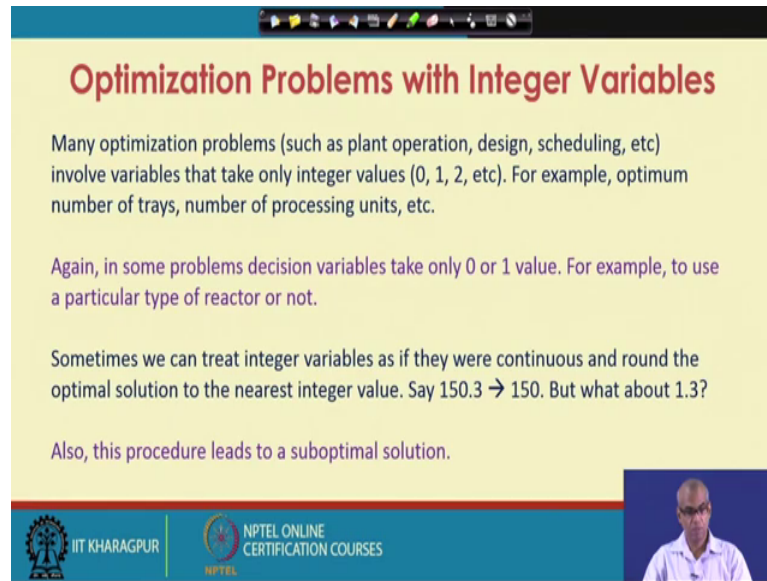
Today's Topic:

An introduction to Solution of Integer Programming Problems

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So, today's topic will be an introduction to solution of Integer programming problem.

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**Optimization Problems with Integer Variables**

Many optimization problems (such as plant operation, design, scheduling, etc) involve variables that take only integer values (0, 1, 2, etc). For example, optimum number of trays, number of processing units, etc.

Again, in some problems decision variables take only 0 or 1 value. For example, to use a particular type of reactor or not.

Sometimes we can treat integer variables as if they were continuous and round the optimal solution to the nearest integer value. Say  $150.3 \rightarrow 150$ . But what about 1.3?

Also, this procedure leads to a suboptimal solution.

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So, what are the problems with integer variables? Many optimization problems such as plant operation, design scheduling etcetera involve variables that take only integer values such as 0 1 2 3 etcetera.

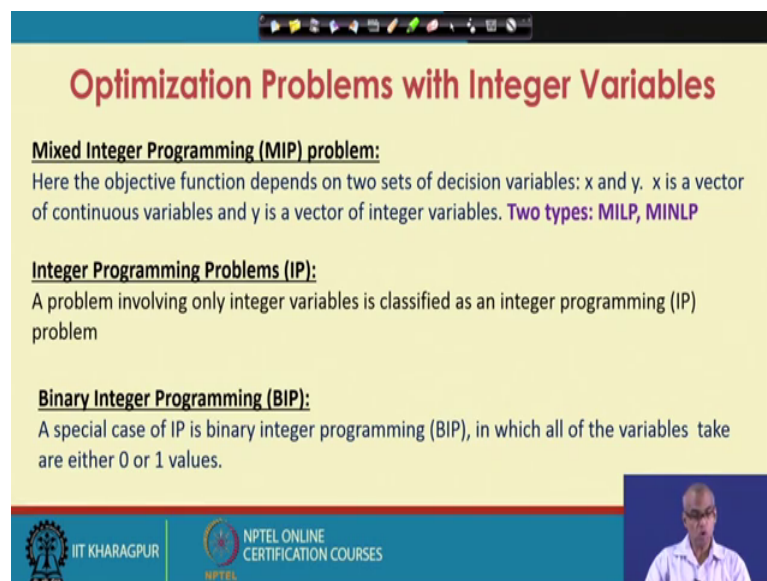
For example, if the decision variables in your optimization problem is number of trays or number of processing units, you are going to get integer values. You are essentially treating them as integer variables. Again in some problems decision variables take only 0 or 1 value for example, whether to install a particular piece of equipment or not whether to use a particular type of reactor or not so, such decisions will be indicated either by 0 or 1.

You can consider 0 for not to use a particular type of reactor and 1 as use a this particular type of reactor. Sometimes we can treat integer variables as if they are continuous and round the optimal solution to the nearest integer value. So, often times we can treat the integer variables as if there continuous and round optimal solution to the nearest integer value.

This perhaps will give you a practical solution when the values of such variables are large. Let us say you are finding out optimal number of trays in distillation column, you treat the variable as continuous variable and get a solution such as 150.3.

So, this you can consider as 150; you can round 150.3 as 150 perhaps without compromising much. But suppose for some other problem you get the optimal value for a decision variables as 1.3. So, here the choices of rounding is not that obvious because 0.3 you can happily neglect considering the number 150, but this choice is not so, obvious when the number is 1.3. So, this procedure of rounding off will lead to some optimal solutions. And strategies and methods have been developed for problems which contain integer variables.

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**Optimization Problems with Integer Variables**

**Mixed Integer Programming (MIP) problem:**  
Here the objective function depends on two sets of decision variables:  $x$  and  $y$ .  $x$  is a vector of continuous variables and  $y$  is a vector of integer variables. **Two types: MILP, MINLP**

**Integer Programming Problems (IP):**  
A problem involving only integer variables is classified as an integer programming (IP) problem

**Binary Integer Programming (BIP):**  
A special case of IP is binary integer programming (BIP), in which all of the variables take are either 0 or 1 values.

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So, let us first look at some of the classifications for those problems which contain integer variables. First mixed integer programming problem is abbreviated as MIP problems. Here the objective functions depends on 2 sets of decision variables  $x$  and  $y$ ;  $x$  is vector of continuous variables and  $y$  is a vector of integer variables.

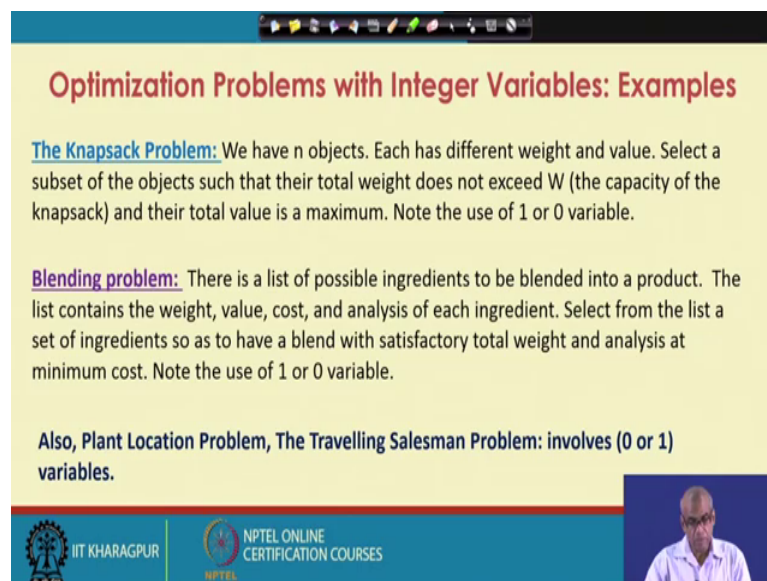
So, if your optimization problems contain both continuous variable and integer variables we call this problem as mixed integer programming problem. Now the mixed integer programming problems can be of 2 types. Mixed integer linear programming, mixed integer non-linear programming. In case of mixed integer linear programming your objective function is linear and all the constraint are linear, but the decision variables can take integer values.

So, the difference between linear programming problem and mixed integer linear programming problem is this that, in case of linear programming problem the decision

variables take on continuous values. And in case of mixed integer linear programming problem the decision variables can take integer values, but in both the cases the objective function on the constants are all linear. In case of mixed integer non linear programming problem it is a non-linear programming problem where the objective function and the constants may be all non-linear additionally the decision variables can take integer values.

So, in case of MILP and MINLP some of the decision variables can take integer values the remaining variables can take continuous values. Integer programming problems are those problems which involve only integer variables. So, they are not mixed integer programming problem they are integer programming problem. So, here all variables contain integer values. Binary integer programming problem is a special case of integer programming problem. Here all the variables take either 0 or 1 values.

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**Optimization Problems with Integer Variables: Examples**

**The Knapsack Problem:** We have  $n$  objects. Each has different weight and value. Select a subset of the objects such that their total weight does not exceed  $W$  (the capacity of the knapsack) and their total value is a maximum. Note the use of 1 or 0 variable.

**Blending problem:** There is a list of possible ingredients to be blended into a product. The list contains the weight, value, cost, and analysis of each ingredient. Select from the list a set of ingredients so as to have a blend with satisfactory total weight and analysis at minimum cost. Note the use of 1 or 0 variable.

Also, Plant Location Problem, The Travelling Salesman Problem: involves (0 or 1) variables.

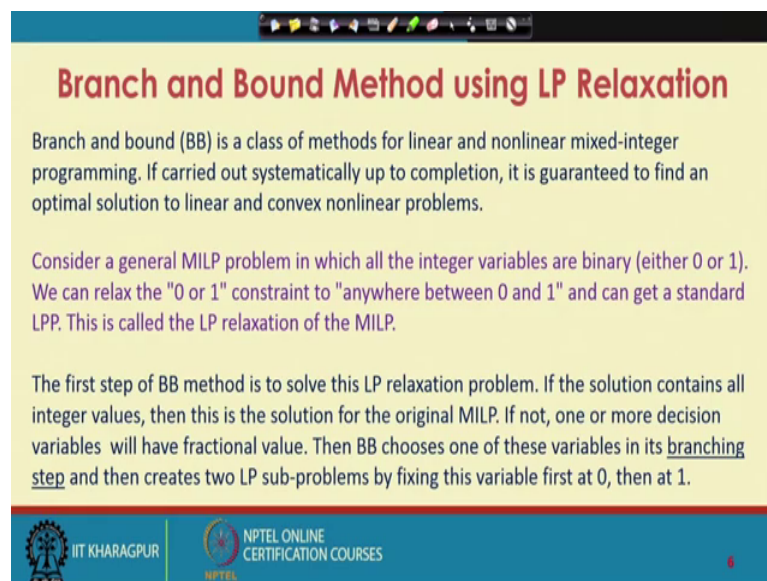
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So, binary integer programming problem contain either 0 or 1 values. Now here is some examples for optimization problems with integer variables. The Knapsack problem we have discussed at the very beginning of this course. Consider you have  $n$  objects and you have to select some of these objects and you will put in your Knapsack. So, you have  $n$  objects each has different weight and value. Select the sub set of the object such that their total weight does not exceed a given value  $W$  which is the capacity of the knapsack and their total value is maximum.

So, basically you have  $n$  objects each object has different weight and different value. So, we have to select a sub set from this  $n$  objects and you will try to maximize the value, but you also have to take care that the total weight of objects does not exceed the capacity of the knapsack. So, note the use of 1 or 0 variable. So, to select the particular object or not to select; if you select we call it 1 if you do not select we assign 0 to it. Similarly blending problem consider that there is a list of possible ingredients to be blended into a product; the list contains the weight value cost and analysis of each ingredient select from the list a set of ingredients.

So, as to have a blend with satisfactory total weight and analysis at minimum cost. Note the use of 1 or 0 variable again. Whether you want to select the particular ingredient or not depending on that you assign either 1 or 0 to that particular variable. Also plant location problem the travelling salesman problem all will involve 0 or 1 variables. So, these are all optimization problems with integer variables particularly 0 1 variable.

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**Branch and Bound Method using LP Relaxation**

Branch and bound (BB) is a class of methods for linear and nonlinear mixed-integer programming. If carried out systematically up to completion, it is guaranteed to find an optimal solution to linear and convex nonlinear problems.

Consider a general MILP problem in which all the integer variables are binary (either 0 or 1). We can relax the "0 or 1" constraint to "anywhere between 0 and 1" and can get a standard LPP. This is called the LP relaxation of the MILP.

The first step of BB method is to solve this LP relaxation problem. If the solution contains all integer values, then this is the solution for the original MILP. If not, one or more decision variables will have fractional value. Then BB chooses one of these variables in its branching step and then creates two LP sub-problems by fixing this variable first at 0, then at 1.

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So, we will now briefly discuss branch and bound method that uses linear programming relaxation for solutions of such integer programming problem or binary integer programming problem or binary integer programming problem.

So, branch and bound is a class of methods for linear and non-linear mixed integer programming problem. So, branch and bound method can solve linear as well as non-linear mixed integer programming problems. So, it is a class of methods. If carried out

systematically up to completion, it is guaranteed to find an optimal solution to linear problems and convex non-linear problems.

So, consider a general mixed integer linear programming problem in which all the integer variables are binary either 0 or 1. We can relax 0 or 1 constraint to anywhere between 0 and 1 and can get standard linear programming problem. If you consider mixed integer linear programming problem, the only difference between mixed integer linear programming problem and standard linear programming problem is this that, in standard linear programming problem the decision variables take on continuous values. And in case of mixed integer linear programming problem the decision variables can take integer values.

So, if you relax this 0 or 1 constraint to anywhere between 0 and 1, I get a standard linear programming problem. This is called the linear programming relaxation of the mixed integer linear programming problem. Note that once you have a standard linear programming problem you can solve it very efficiently. Using simplex method you can make now use of (Refer Time: 13:20) that you are familiar with you are now also familiar with `xlsolver` and you can use this Matlab program Matlab optimization tool box or excel solver for solution of linear programming problems. The first step of branch and bound method is to solve this linear programming relaxation problem. If the solution contains all integer values then this is the solution for the original mixed integer linear programming problem.

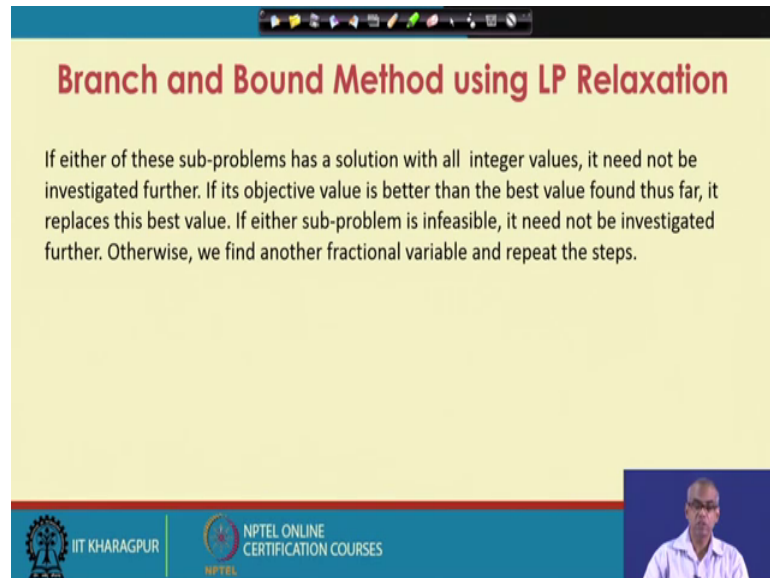
So, you do not have to do anything next. You have already obtained the solution, but if the solution that does not contain all integer values it means 1 or more decision variables have fractional values. So, one or more decision variables have fractional values then branch and bound chooses one of these variables in its branching step and then creates 2 linear programming sub problems by fixing this variable first at 0 then at 1.

So, we repeat the first step of branch and bound method is to solve this linear programming relaxation. If the solution contains all integer values.

Then this is the solution for the original mixed integer linear programming problem, but if the solution does not contain all integer values it means 1 or more decision variables have fractional values. Then branch and bound chooses one of these variables which has

fractional values in it is branching step and then creates 2 linear programming sub problems by fixing this fractional value first at 0 then at 1.

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**Branch and Bound Method using LP Relaxation**

If either of these sub-problems has a solution with all integer values, it need not be investigated further. If its objective value is better than the best value found thus far, it replaces this best value. If either sub-problem is infeasible, it need not be investigated further. Otherwise, we find another fractional variable and repeat the steps.

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If either of these sub problems has a solution with all integer values it need not be investigated further. If it is objective value is better than best value found thus far it replaces this best value. If either sub problem infeasible it need not be investigated further. Otherwise we find another fractional variable and repeat the steps.

So, this is the steps you have to follow to solve a mixed integer linear programming problem using branch and bound method.



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**Binary Integer Programming Problems: Branch and Bound Method using LP Relaxation: Example**

Maximize  $f = 86x_1 + 4x_2 + 40x_3$   
Subject to:  $774x_1 + 76x_2 + 42x_3 \leq 875$   
 $67x_1 + 27x_2 + 53x_3 \leq 875$   
 $x_1, x_2, x_3 = (0,1)$

Edgar, Himmelblau, and Lasdon (2<sup>nd</sup> Edition)

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So, let us now take one example from the text book and we solve using branch and bound method using linear programming relaxation. So, you have been given a linear programming problem. So, what is the first step? First step is to solve a L P relaxation.

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**Branch and Bound Method**

Upper bound = 129.1  
Lower bound =  $-\infty$   
No incumbent

Continuous LP optimum  
 $0 \leq x_1 \leq 1$   
 $0 \leq x_2 \leq 1$   
 $0 \leq x_3 \leq 1$   
 $x^* = (1, 0.776, 1)$   
 $f = 129.10$

The first step is to solve the LP relaxation of the binary IP. The optimal solution has one fractional (non-integer) variable ( $x_2$ ) and an objective function value of 129.1.

Because the feasible region of the relaxed problem includes the feasible region of the initial IP problem, 129.1 is an upper bound on the value of the objective function of the IP.

The lower bound is set to  $-\infty$ .

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So, the first step is to solve the L P relaxation of the binary integer programming problem. Note that this is binary integer programming problem all  $x_1$ ,  $x_2$  and  $x_3$  can take either 0 or 1. Now the first step is to solve the L P relaxation of the binary integer programming problem.



So, you can solve this. How do you obtain this L P relaxation simply by considering  $x_1$ ,  $x_2$  and  $x_3$ . They all lie between 0 and 1 anywhere between 0 and 1 not just either 0 or 1. So, this is the L P relaxation.

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**Binary Integer Programming Problems: Branch and Bound Method using LP Relaxation: Example**

Maximize  $f = 86x_1 + 4x_2 + 40x_3$

Subject to:  $774x_1 + 76x_2 + 42x_3 \leq 875$

$67x_1 + 27x_2 + 53x_3 \leq 875$

$x_1, x_2, x_3 \in \{0,1\}$

$0 \leq x_1, x_2, x_3 \leq 1$

Edgar, Himmelblau, and Lasdon (2<sup>nd</sup> Edition)

So, if you replace the 0 1 constant by this please note that you have a regular standard linear programming problem. Which can be solved using any solver such as Matlab (Refer Time: 18:06) or excel solver for simple problems you can do hand computation using simplex method, but it will be more convenient to make use of Matlab tool box or excel solver.

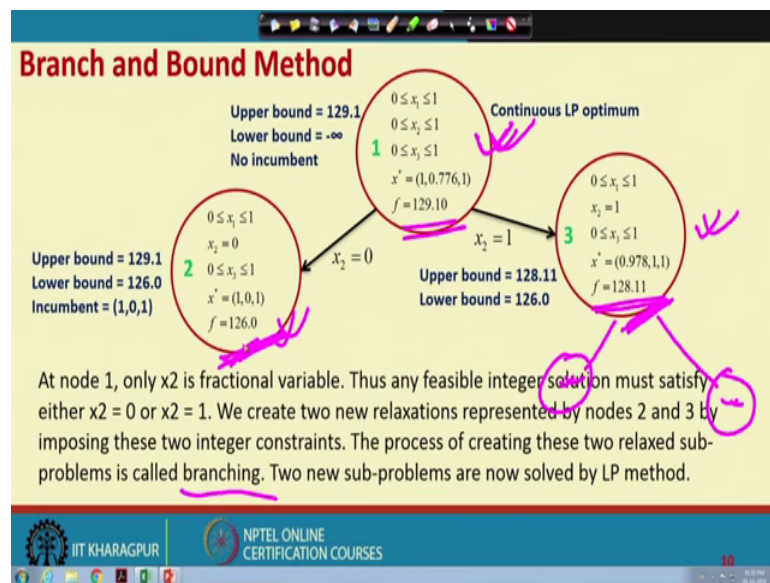
So, first step is to solve the L P relaxation. The optimal solution is this. Note that in the optimal solution  $x_1$  is integer to it is fractional and  $x_3$  is integer. And the objective value function is 129.10 because the feasible region of the relaxed problem include the feasible region of the initial integer programming problem. The optimal solution 129.10 is a upper bound on the value of the objective function of the original integer programming problem.

So, integer programming problem has restrictions on decision variables as either 0 or 1. And the linear programming problem has anywhere between 0 and 1. So, the feasible region of the relaxed problem that is the linear programming problem includes the feasible region of the original integer programming problem.

So, therefore, the optimal solution that, I get using the relaxed linear programming problem is an upper bound on the value of the objective function of the integer programming problem.

So, the upper bound set is 129.10. I do not have any feasible solution known to figure out what may be the lower bound. So, I set the lower bound as minus infinity. So, now, look at the optimal solution 2 integer values, but  $x_2$  is fractional.

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So, only  $x_2$  is fractional variable at node 1. So, thus any feasible integer solution must satisfy either  $x_2$  equal to 0 or  $x_2$  equal to 1. At node 1  $x_2$  is obtained as 0.776. So, any feasible integer solution must satisfy either  $x_2$  equal to 0 or  $x_2$  equal to 1.

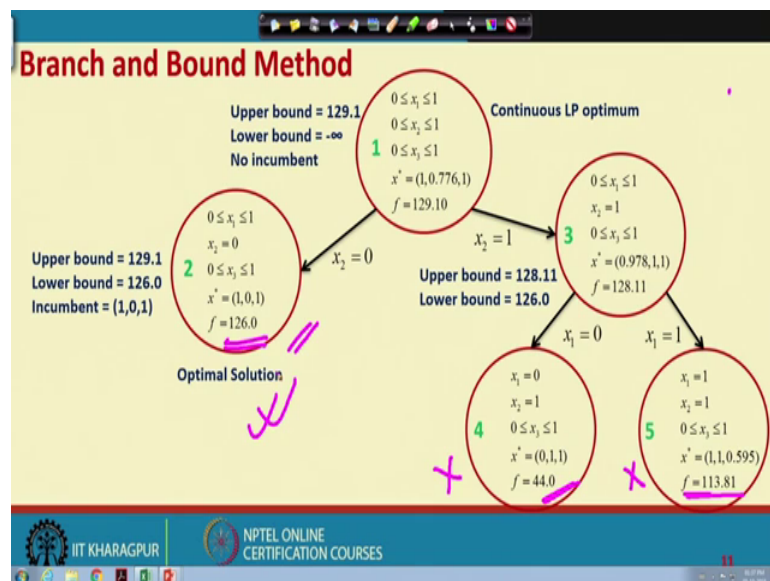
So, you can create 2 new relaxation represented by node 2 and nodes 3 by imposing these 2 integer constraint. So, at node 2 I let  $x_1$  vary between 0 and 1.  $x_3$  vary between 0 and 1, but  $x_2$  I set as 0. Similarly at node 3 I said  $x_2$  at 1, but  $x_1$  and  $x_3$  vary between 0 2 1.

So, we created two new relaxations at nodes 2 and node 3 by imposing integer constant. The process of creating this two relaxed sub problems is called branching. This is what we call branching. So, node 1 now had just 2 branches node 2 and node 3. So, solve these 2 new sub problems again you can use any solver to solve these problems.

So, when all these sub problem at node 2 I get all the values as integer at optimal solution 1 0 1 is the solution solve integer values and objective function values is 126. And node 3, I have  $x_1$  as fractional values  $x_2$  and  $x_3$  are integer and the objective function value is 128. Note that the branches that I get from any node cannot have an optimal solution which is better than this node. So, that is why you get 129 here, but here we get 126 here we get 128.

So, these does not contain any fractional value. So, we are done this node, but this node contains 1 fractional value. And also the optimal value here is 128.11. So, I must get another 2 branches from here because these 2 nodes may have a solution which is 120.11 or less than that, but that may be higher than 126. So, I must consider branching of node 3 note that branching of node 2 is not required any more.

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So, again I made 2 branches; branch node 4 and node 5. Node 4 again I got all integer solutions with objective function value 44. So, node 4 no more branching required. Node 5 the optimal solutions contain 2 integer values 1 continuous value, but it objective function value is 113. The objective function value is 113.81. So, if I take branches from node 5.

If I create node 6 and node 7 from node 5 the optimal values of those sub problems will have the objective function value either 113.81 or less than that which is less than 126. So, here also no more branching required here also no more branching required. Now

compare this and this because these are the 2 cases where I have all the decision variables as integer variables. Obviously, this one is the optimal solution. Note that your maximizing the objective function.

So, node 2 contains the optimal solution. So, the optimal solution says  $x_1$  equal to 1  $x_2$  equal to 0 and  $x_3$  equal to 1. And the optimal values of the objective function is 126. So, this is how you can solve a binary integer programming problem using branch and bound method. The branch and bound method is very interesting and very robust method. The problem that will appear is as the size of the problem increases you can expect that the number of such branches or the decision tree that will be huge, but if you carry out all the computations till completion systematically you are guaranteed to get the optimal solution.

So, this brings us to the end of this course. In this course I have tried to give you abroad overview of various optimization techniques that are available for solutions of constraint and unconstrained optimization problems.

So, we started with formulation of optimization problems we talked about formulation of various optimization problems. Then we talked about optimality conditions for unconstrained optimization problems and constrained optimization problems.

We learnt about (Refer Time: 28:32) conditions. Then we discussed methods for solutions of single variable unconstrained optimization problems multi variable unconstrained optimization problems. Then we talked about linear programming problems we talked about non-linear programming problems with constraints and then we talked about various optimization problems that you may encounter in the field of discipline chemical engineering or bio chemical engineering. And finally, we talked about software tools for solutions of optimization problems.

In particular we have seen applications of Matlab optimization tool box and Microsoft excel solver for solution of optimization problems. With this note I would like to close it is course. I hope that this course will be useful to you and you have enjoyed the course I wish you good luck for you exam.

Thanks for attending my course.