Optimization in Chemical Engineering
Prof. Debasis Sarkar
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur

Lecture – 47
Constrained Nonlinear Programming (Contd.)

Welcome to lecture 47, this is week 10 and we were talking about Constraint Non-linear Programming in this week. In our previous lecture we have talked about successive linear programming for solution of non-linear programming problems. In today's lecture we will talk about a similar method and this is successive quadratic programming approximation of a general non-linear programming problem and a solution method based on that.

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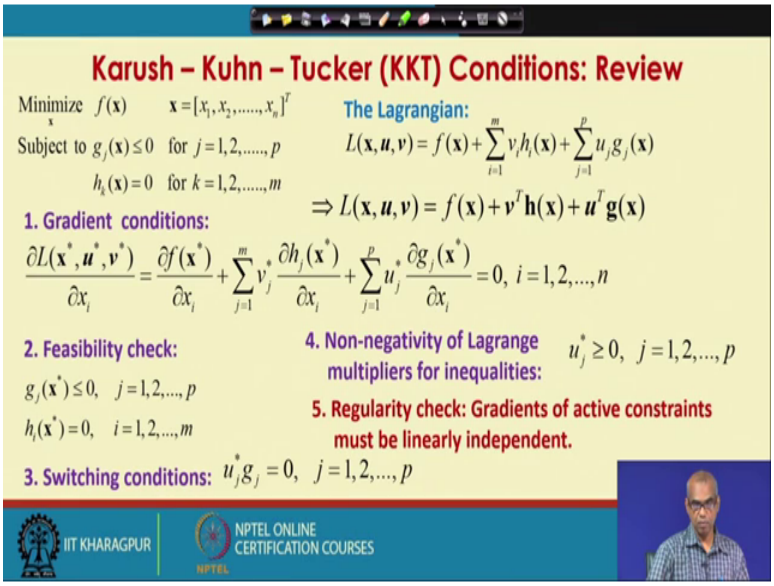

So, again we start with a brief review of KKT conditions we will make use of KKT conditions in today's lecture. So, we have a general non-linear programming problem minimization of objective function f x, which is the function of n variables subject to p inequality constraints all are less or equal to type and m number of equality constraints.

So, we first formulate the Lagrangian, define Lagrange multiplier and KKT multiplayer for each of the constraints and then formulate the Lagrangian. The Gradient conditions which is del l del xi equal to 0. So, this will lead to n equations corresponding to n decision variables. Feasibility check, which says that the inequality constrained and the equality constraints must be satisfied. Switching conditions, which says the product of Lagrange multiplier or the KKT multiplier with the inequality constrained will be equal to 0. Non- negativity of Lagrange multipliers for inequality constraints and finally, regularity check which says the gradients of active constraints must be linearly independent.

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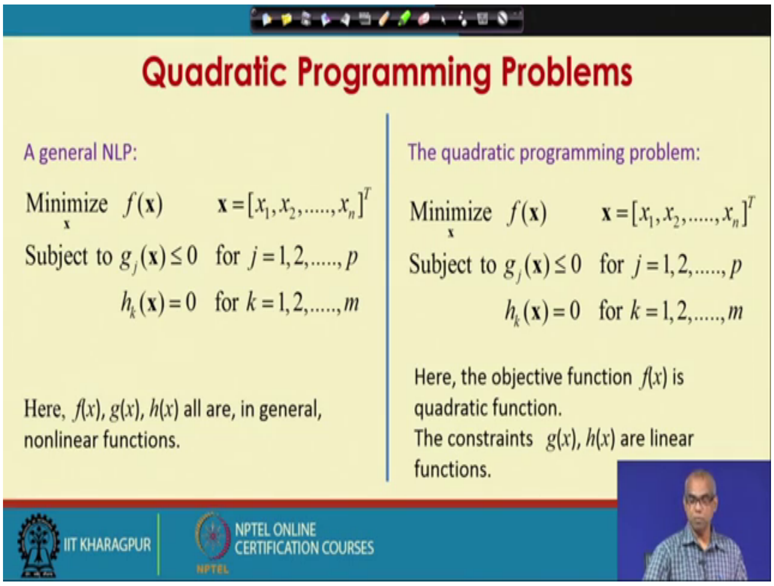

Now, let us first talk about quadratic programming problems. We are familiar with the structure of a general non-linear programming problem. In general in a non-linear programming problem you will have an objective function which is non-linear and inequality constraints and the equality constraints are all non-linear functions of decision variables. We have seen in case of linear programming, problem the objective function and all the constraints are linear functions of decision variable. In case of quadratic programming problem the objective function is a quadratic function, but the constraints are all linear functions.

So, quadratic programming problem the objective function is a quadratic function, but all the constraints are linear. So, quadratic programming problem has a special form where the objective function is non-linear, but to the extent that it is a quadratic function and similar to linear programming problem all the constraints are linear functions. So, perhaps we can intuitively think at this stage that it may be possible to solve a quadratic programming problem by use of a linear programming problem. The way we have solve linear programming problem maybe it is possible by some modifications we will also be able to solve the quadratic programming problem following the method of solution of linear programming problem.

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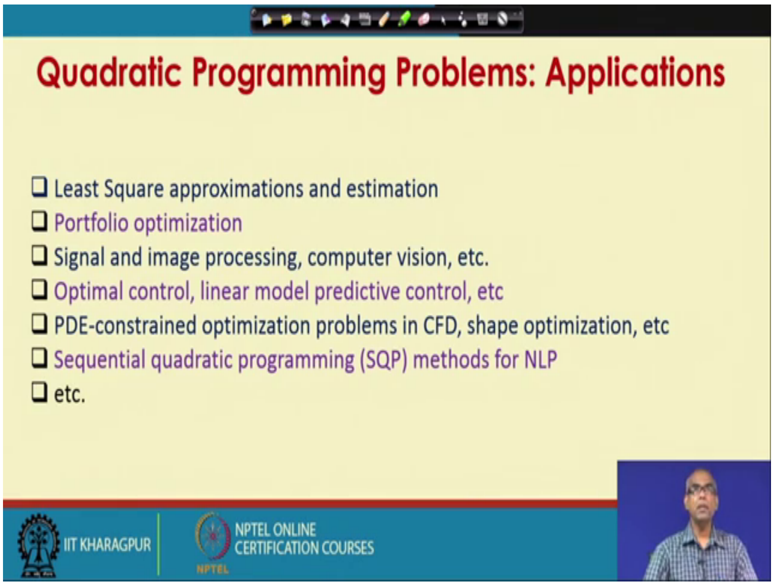

There are various applications of linear programming problems, sorry there are various applications for quadratic programming problems some of them are listed here least square approximation and estimation. The least square approximations and estimation lead to a quadratic programming problem, portfolio optimization, signal and image processing, computer vision etcetera, optimal control, linear model predictive control, Partial Differential Equation- constrained optimization problems in Computational Fluid Dynamics, shape optimization, sequential quadratic programming methods for solution of Non-Linear Programming problems etcetera.

So, there are various interesting applications of quadratic programming problems some of those are listed here.

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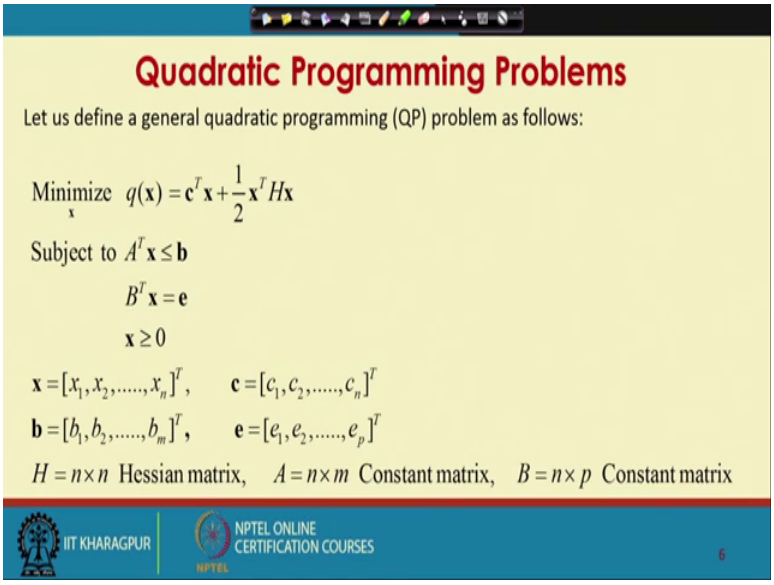

So, let us now define a general quadratic programming problem, as you have mentioned that for a quadratic programming problem the objective function is the quadratic function. So, we can note that the objective function here is c transpose x plus half x transpose Hx which you know that is a standard expression of a quadratic function.

Here c is an n vector, x is also n vector, each component is decision variables so, there n decision variables and c are the corresponding coefficients. So, it is like c 1 x 1 plus c 2 x 2 like that. So, c transpose x will lead to an equation like that, H is n cross n Hessian matrix. So, this is about the objective function which is a quadratic in x, subject to set of inequality and equality constraints and they are all linear.

So, the inequality constrained is written as A transpose x less or equal to b, where b is m vector. So, basically you will have A matrix, you will have x vector and then you will have b vector. So, A is n cross m constrained matrix and this is n vector, next you have a set of equality constrained. Similarly equality constraints are written as B transpose x equal to e, where B is the constrained matrix n cross p and e is a p vector which represents the right hand side.

So, A transpose x less or equal to b, b represents the right had side vector, B transpose x equal to e, e represents the right hand side vector and non negativity constrained on the decision variables. So, this is a general formulation of a quadratic programming problem where you have the objective function is a quadratic function c transpose x plus half x transpose Hx subject to A transpose x less or equal to b as in equality constrained B transpose x equal to e as equality constraints and the non negativity constraints on decision variable x which is written as x greater equal to 0.

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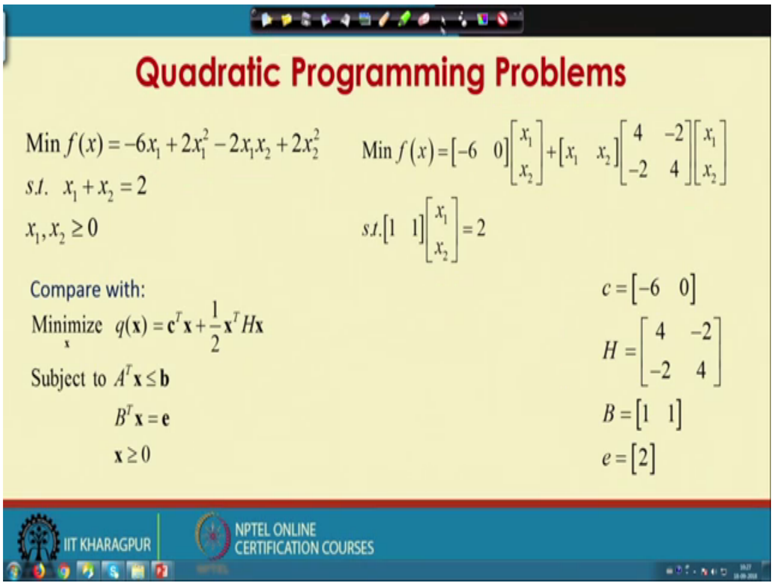

So, let us take an example, objective function is given as minus 6x 1 plus 2x 1 square minus 2x 1 x 2 plus 2x 2 square subject to x 1 plus x 2 equal to 2 and x 1 x 2 both are nonnegative. The objective function is a quadratic function compare now, with the general form. So, can you rewrite this equations into this form we can do that you need to identify that this expressions can be written as this note this part is c transpose x and this part is x transpose Hx, x is the n vector. So, x transposes is rho vector. So, x transpose Hx and c transpose x with help of that you can re write this original quadratic equation.

Similarly, x 1 plus x 2 equal to 2 can also be written as B transpose x equal to 2 note that c H B e are identified as shown. So, I will suggest you take similar such expressions and try to rewrite them in the standard form; that means, right in the form c transpose x plus half x transpose a Hx for the objective function. So, identify c and H and depending on whether you have equality constraints, inequality constraints or both you try to identify A and B and also write the constraints in the matrix notation.

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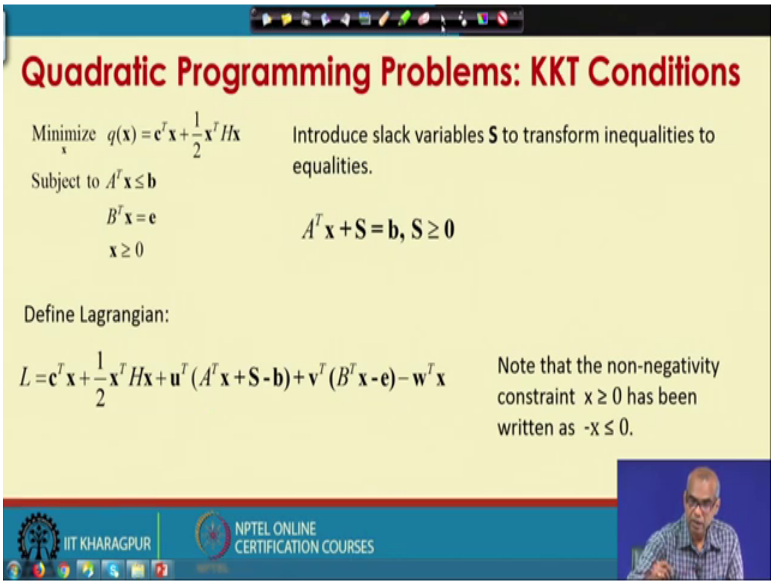

So, now let us write down the KKT conditions for the quadratic programming problems. So, the first thing is to introduce the slack variable to transform the inequality constraints to equality constraints, A transpose x less or equal to b or my inequality constraints. So, let us introduce slack variables S to each of these inequality constraints and in vector matrix notation we can write A transpose x plus S equal to b an S is non 0 sorry S is non negative. We know that the slack variables will be non negative. So, note that S is a vector. So, we have now converted then equality constraints to equality constraints. So, I now have a objective function which is quadratic and all the constraints which are of equality type.

So, let us now define the Lagrangian. So, the Lagrangian is define following the usual practice this is my equality constraints which are transformed from the inequality constraints. So, in the Lagrangian formulation I have u as multipliers. So, u transpose into A transpose x plus S minus b, this term I get for this equality constraints. Similarly for the original equality constraints in the original problem v transpose x equal to e gets reflected in the Lagrangian as v transpose into B transpose x minus e.

And then finally, x greater or equal to 0 is written as minus x less or equal to 0 and I define the multiplied w. So, this becomes minus w transpose x and we add all these thing terms to the objective function c transpose x plus half x transpose Hx. So, this is how the Lagrangian is formulated, the objective function these are the inequality constraints which I converted to equality constrained by addition of slack variables. This is for the equality constraints which are already present in the original quadratic programming problem and this is due to non negativity restrictions on the decision variables. So, once I have this Lagrangian I can now apply the first order optimality conditions or we can write down the KKT conditions.

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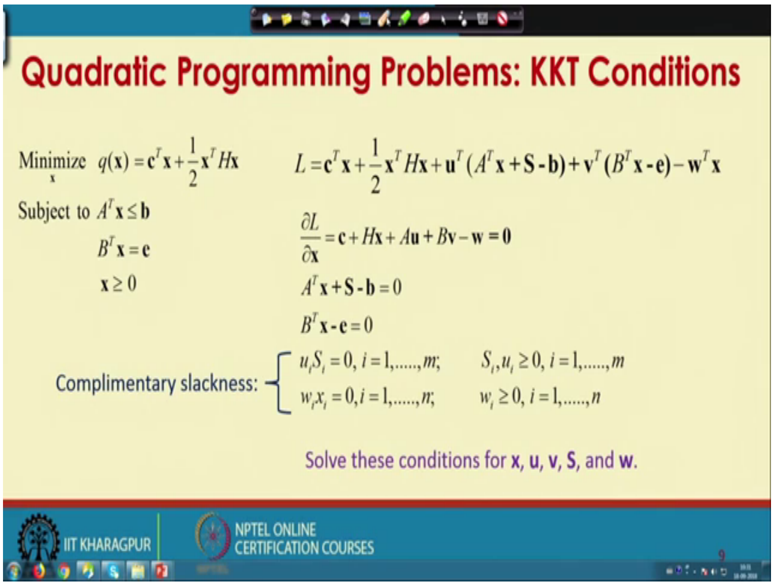

So, the KKT conditions we write down now, first is the gradient of the Lagrangian with respect to the decision variables equal to 0. So, this gives me this expression. So, this is Lagrangian take the derivative of L with respect to each decision variable.

So, if you do that I get c from this term, I get Hx from this term, I get A u from this term, I get B v from this term and I get minus w from this term, note that this is a linear expression. And then you have the feasibility check so, this was gradient condition, this is the feasibility check the feasibility check says that these constraints must be satisfied. So, A transpose x plus S minus b equal to 0, B transpose x minus e equal to 0. And then the complementary slackness which says u i S i equal to 0 for i equal to 1 to m and w i x i equal to 0 for i equal to 1 to n. Note that there are n number of constraints in equality constraints note that there are n number of inequality constraints. So, for each of them you need slack variables.

So, these leads to u i S i equal to 0 and this n decision variables needs w i x i equal to 0 for i equal to 1 to n, note that S i u i and w i are all constrained to be greater or equal to 0, the slack variables and the Lagrangian multipliers for the inequality constraints are nonnegative. So, that is why this grater or equal to 0 terms here. So, now, we can solve this conditions for x, u, v, s and w that will give me the KKT point and that maybe a candidate for optimal point.

So, now we have seen that these are basically linear equations, this is linear and these were already linear. So, now, this can these equations can be written in a compact form using matrix notations. So, let us see how we will do that.

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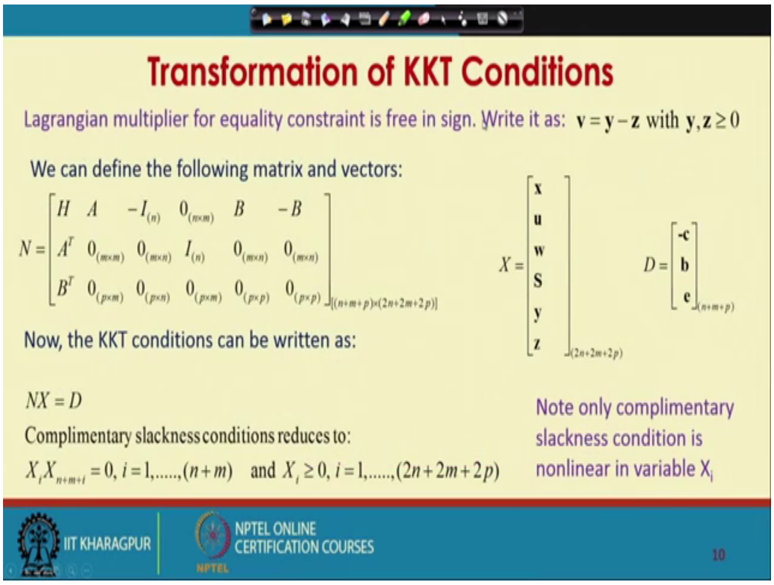

So, before doing that let us identify that the Lagrange multipliers for the equality constraint; that means, these v are free in sign, in other words they can take both positive and negative values.

So, we can express them as the difference of 2 non negative terms. So, this is what we do. So, replace v as y minus z with y greater equal to 0, z greater equal to 0, but u at the Lagrange multipliers for inequality constraints and they are already greater equal to 0. So, now, this I define X as a vector which contains all these variables decision variables, the Lagrangian multipliers, for the in equality constraints, the w for the x greater equal to 0, the slack variables and y and z that replaces v. So, I can define a vector of size 2 n plus 2 m plus 2 p.

Similarly I define a D vector which is minus c b and e as components. So, it is n plus m plus p vector. Now if we define an N matrix using H as a Hessian matrix A and B and identity matrix and null matrix I basically represents the linear systems of equations that we obtained when you applied the KKT conditions; that means, these set of equations.

So, these set of linear systems can be represented in matrix notations using this definition of N, this definition of X and this definition of D, by NX equal to D. So, those KKT conditions the linear systems corresponding to KKT conditions can be written as NX equal to D, where N is this matrix, X and D are this vector and this vector respectively. The complementary slackness which are u i S i equal to 0 and w i x i equal to 0 can be written as X i X n plus m plus i equal to 0, for i equal to 1 to n plus m and X i grater equal to 0 for i equal to 1 to 2 n plus 2 m plus 2 p, note that this is capital X.

So, this capital X is a vector with the decision variable vector X u w s y and z. So, now, if you look at these set of equations NX equal to D and this new complementary slackness condition we see that except this complementary slackness conditions I have a linear set of linear systems I have a set of linear systems only the complementary slackness condition is non-linear in variable X i.

So, the solution to NX equal to D if that solution satisfies the complementary slackness condition then it becomes a solution to the KKT point or solution to the original Quadratic Programming problem. So, I repeat the KKT conditions of the Quadratic Programming problem can be written as NX equal to D which is a set of linear systems, which is a set of linear equations, the complementary slackness condition is non-linear. So, the solutions of NX equal to D, if the solution of NX equal to D satisfies the complementary slackness condition, then the solution become a KKT point and this becomes a solution to the original Quadratic Programming problem.

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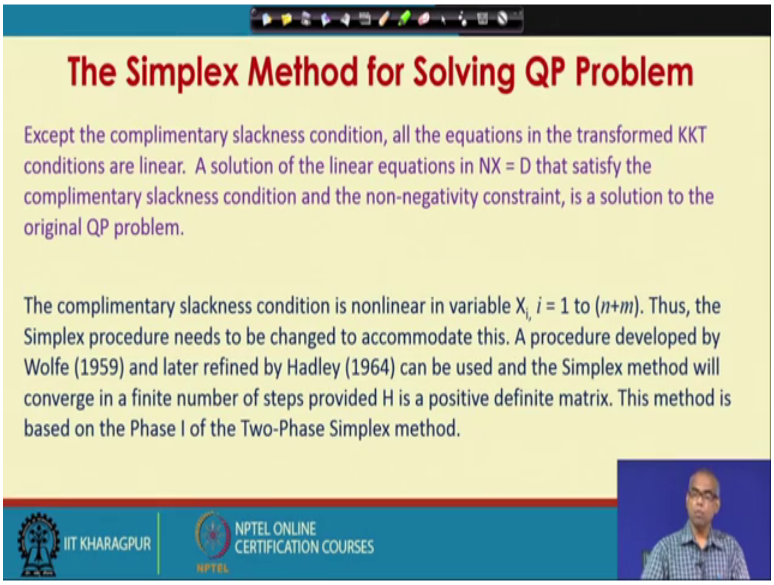

So, except the complementary slackness condition, all the equations in the transformed KKT conditions are linear. A solution of the linear equations in NX equal to D that satisfy the complementary slackness condition and the non negativity constraint, is a solution to the original quadratic programming problem.

The complementary slackness condition is non-linear in variable X i, i equal to 1 to n plus same. Thus, the simplest procedure needs to be changed to accommodate this. A procedure developed by Wolfe and later refined by Hadley can be used and the Simplex method will converge in a finite number of steps provided the Hessian matrix H is a positive definite matrix. This method is based on the phase one of the two- Phase Simplex Method that you have discussed earlier.

So, what we get it is that. The solution to the set of equation NX equal to D we need to find out and if that solution satisfies the complementary slackness condition I have a solution to the original programming problem. Now since the complementary slackness condition is non-linear the regular simplex method needs to be modified, that modification has been proposed by Wolfe and Hadley and the modified method can be used and the Simplex method then converges in a finite number of steps provided the Hessian matrixes of a positive definite matrix. So, we can conclude that the quadratic programming problem can be solved using a Simplex method where the Simplex method needs to be modified to accommodate the non-linear complementary slackness conditions.

So, let us assume that we are able to solve a quadratic programming problem with non-linear complementary slackness condition by modified simplex method. So, then we know how to solve a quadratic programming problem.

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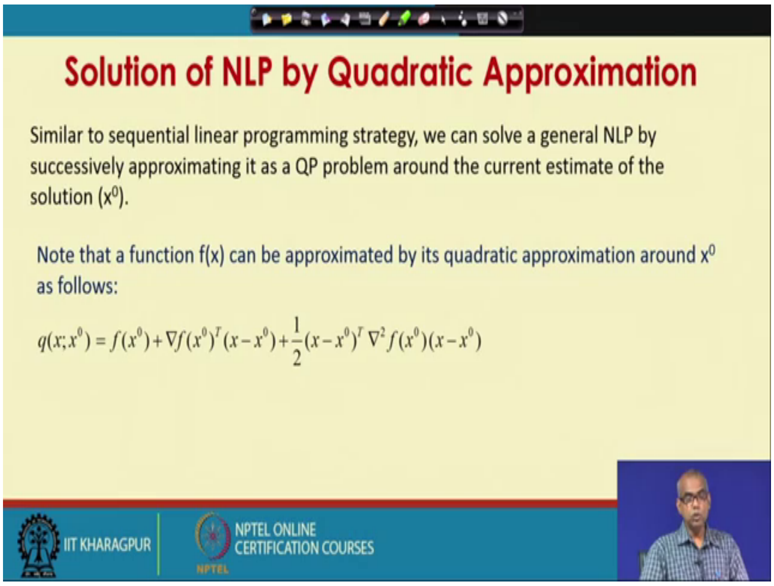

So, similar to sequential linear programming strategy we can now solve a general non-linear programming problem by successively approximating it as a quadratic programming problem around the current estimate of the solution. Similar to sequential linear programming strategy we can solve a general non-linear programming problem by successively approximating it as a quadratic programming problem around the current estimate of the solution x 0, note that a function f x can be approximated by quadratic approximation around x 0 as shown.

So, this is f of x 0 plus gradient of f at x 0 into x minus x 0 plus half x minus x 0 transpose Hessian evaluated x 0 into x minus x 0. So, any function f x can be approximated by it is quadratic approximation which is this.

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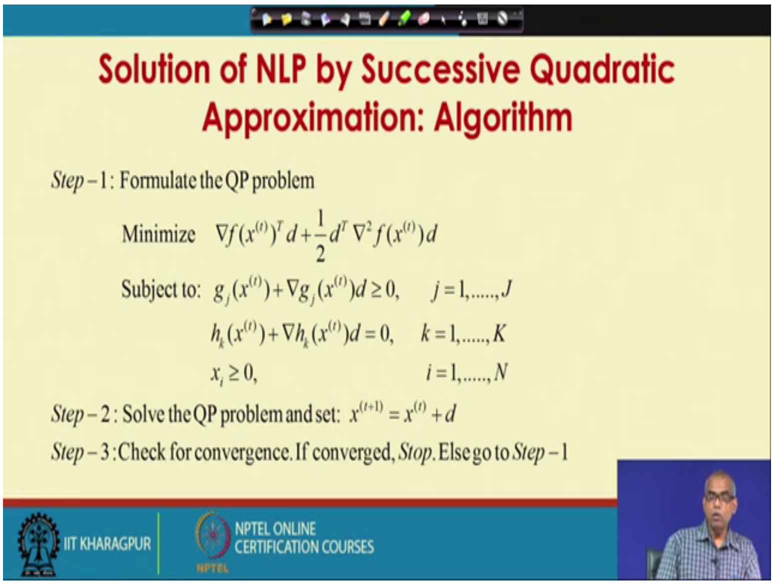

So, we now give the algorithm for successive quadratic approximation. So, formulate the quadratic programming problem as shown; that means, the objective function is the quadratic function and note that the constraints has been converted to linear functions by performing Taylor series expansion this we have learnt during successive linear programming.

So, the inequality constraints and the inequality constraints all are linearized by Taylor series expansion. So, this is the quadratic formulation. So, the quadratic objective function linearized inequality constrained by Taylor series expansion and retuning only first order term and also the equality constraints linearized equality constrained by Taylor series expansion retaining the first order term and the non negativity restrictions.

So, we solve now the quadratic programming problem and set the next estimate of the solution as x t plus 1 equal to x t plus d. So, this d is like x minus x 0 that you have seen in the previous slide.

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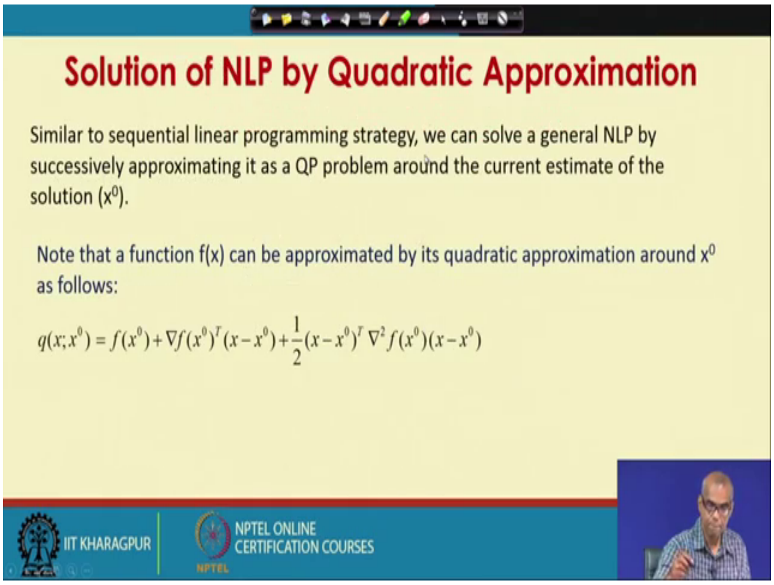

So, now, we check for the convergence in the step 3 if conversely stop otherwise you go to step 1; that means, with the current estimate again we reinitialize the quadratic programming problem and solve again and continue until we converge.

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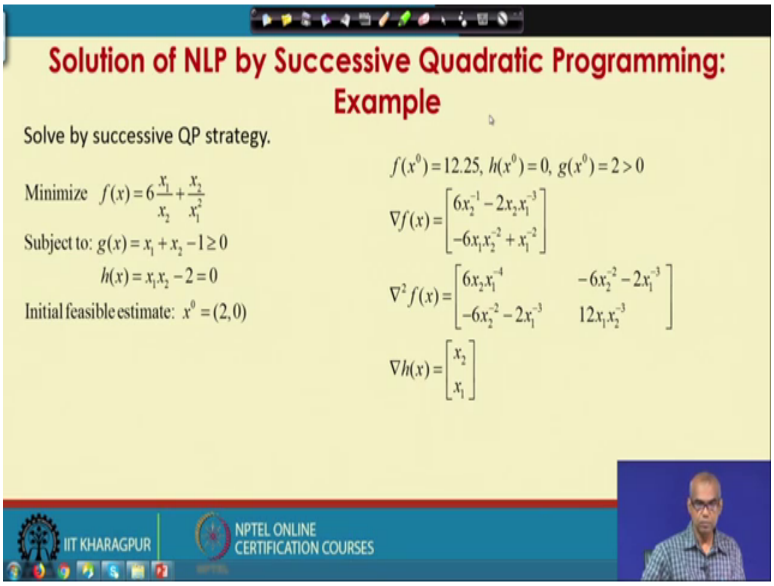

So, now let us take an example. So, you want to solve the problem 6 x 1 by x 2 plus x 2 by x 1 square and g equal to x 1 plus x 2 minus 1 grater equal to 0, h equal to x 1 x 2 minus 2 equal to 0. So, you have equality constraints as non-linear objective function as non-linear. So, we start with an initial feasible estimate of x 0 equal to 2, 0 that mean x 1 equal to 2, x equal to 0.

So, find out the function value add x 1 equal to 2 x 2 equal to 0 find out the value of the objective function and find out the value of the constraints h at x equal to x 0 equal to 0 g at x 0 equal to 2. So, h is greater than 0 the point is feasible. So, evaluate the gradient write down the expression for the gradient hessian and the gradient of the equality constrained, note that in equality constrained is already linear.

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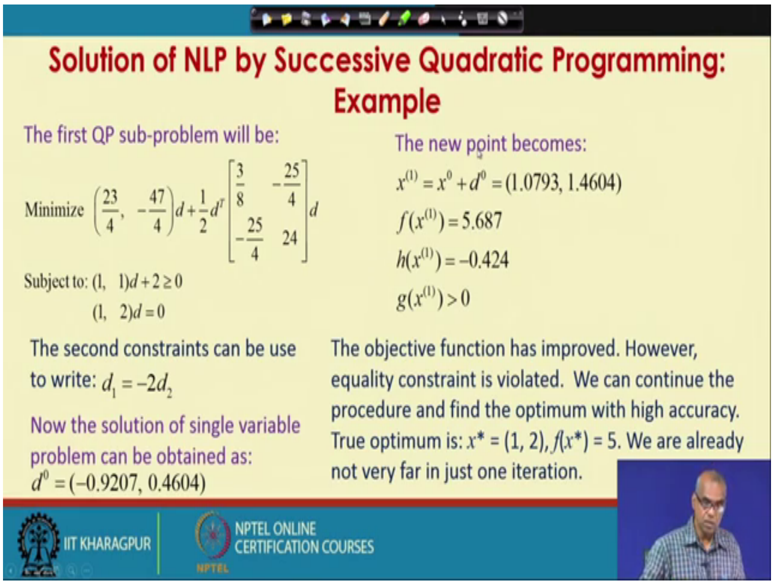

So, you can write down the first quadratic programming sub problem as this, note this is coming from this. The gradient of f the gradient of the objective function evaluated the current estimate in to d plus half transpose Hessian evaluated at current estimate in to d. So, you make use of these to write this.

So, this is the gradient of the objective function evaluate at the current estimate 2 0, this is Hessian evaluated at point 2 0 and inequality constrained linearized equality constraints. Now, the second constrained this you can use to write d 1 equal to minus 2d 2. So, you can express any of this d 1 or d 2 in terms of the other one, note that d is a vector with components d 1 and d 2.

So, d 1 can be written as minus 2d 2. So, then the solution of the single variable problem can be obtained analytically. So, note that this is you have compare it with c transpose x plus half x transpose hx, here x is d, d has components d 1 and d 2. Now once I express d 1 as minus 2d 2, I have a single variable problem this can be solved analytically I get the solution as d 0 equal to minus 0.9207, 0.4604. So, once I have the solution d 0, I can get the new point x 1 as x 0 plus d 0 which is 1.0793, 1.4604 as x 1 x 2. So, this is x 1, this is x 2.

So, this has components like this. So, evaluate the function 5.687, equality constraint is minus 0.424, inequality constraint is greater than 0. So, the equality constraint is violated, objective function is improved. So, you have to continue the procedure and then you can find the optimum with high accuracy; the true optimum is x 1 equal to 1, x 2 equal to 2, objective function equal to 5.

So, we are already the objective function value at 5.687. So, if you do the next iteration you will see that you have obtained the solution with high accuracy very close to 5. So, how will you do that? We have now the value x 1 as 1.0793, 1.4604 so, with this estimate again you have to reinitialize the problem; that means, you have to put the values of x 1 and x 2 in these.

And, then you will write the problem in this form; that means, you will obtain the second quadratic programming sub problem and then you will solve for d you will solve for d 1, then you will solve for x 2 which will be x of 1 and d of 1. So, that solution we will see that is very close to true solution 1 2 and the objective function value will also be very close to 5. So, this is how you will be able to solve a general non-linear programming problem using successive quadratic programming. With this we stop lecture 47 here.