

Optimization in Chemical Engineering
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Lecture – 46
Constrained Nonlinear Programming

Welcome to lecture 46, this is the first lecture of week 10. In this week 10, we will talk about Constrained Non-Linear Programming. As of now, we have talked about optimality conditions for single variable unconstrained problem, multi variable unconstrained problem, constrained problems. We have seen how to solve unconstrained single variable and multivariable problems. We have also seen how to solve Linear Programming Problems.

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Constrained Nonlinear Programming

<u>Week 10:</u>	<u>Today's Topic:</u>
➤ Sequential Linear Programming Method	➤ Sequential Linear Programming Method
➤ Successive Quadratic Programming Method	
➤ Penalty Function Method	
➤ Lagrange Multiplier method	

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In this week, we will see how to solve a general Constrained Non-Linear Programming problem. So, there are various methods of solving a Constrained Non-Linear Programming problem. Some of the methods that we will talk about are Sequential Linear Programming Method, Successive Quadratic Programming Method, Penalty Function Method and Lagrange multiplier method.

So, today we will learn about Sequential Linear Programming method. And as the name suggest a Non-linear programming problem will be solved by a series of solving Linear programming problems.

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Karush - Kuhn - Tucker (KKT) Conditions: Review

Minimize $f(\mathbf{x})$ $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$ **The Lagrangian:**

Subject to $g_j(\mathbf{x}) \leq 0$ for $j=1, 2, \dots, p$ $L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = f(\mathbf{x}) + \sum_{i=1}^m v_i h_i(\mathbf{x}) + \sum_{j=1}^p u_j g_j(\mathbf{x})$

$h_k(\mathbf{x}) = 0$ for $k=1, 2, \dots, m$ $\Rightarrow L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = f(\mathbf{x}) + \mathbf{v}^T \mathbf{h}(\mathbf{x}) + \mathbf{u}^T \mathbf{g}(\mathbf{x})$

1. Gradient conditions:

$$\frac{\partial L(\mathbf{x}^*, \mathbf{u}^*, \mathbf{v}^*)}{\partial x_i} = \frac{\partial f(\mathbf{x}^*)}{\partial x_i} + \sum_{j=1}^m v_j^* \frac{\partial h_j(\mathbf{x}^*)}{\partial x_i} + \sum_{j=1}^p u_j^* \frac{\partial g_j(\mathbf{x}^*)}{\partial x_i} = 0, \quad i=1, 2, \dots, n$$

2. Feasibility check: **4. Non-negativity of Lagrange multipliers for inequalities:** $u_j^* \geq 0, \quad j=1, 2, \dots, p$

$g_j(\mathbf{x}^*) \leq 0, \quad j=1, 2, \dots, p$

$h_k(\mathbf{x}^*) = 0, \quad i=1, 2, \dots, m$ **5. Regularity check: Gradients of active constraints must be linearly independent.**

3. Switching conditions: $u_j^* g_j = 0, \quad j=1, 2, \dots, p$

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So, before we start solving constrained non-linear programming problem, let us first review the KKT conditions or Karush Kuhn Tucker conditions for a general non-linear programming problem. What you see is the statement of a general non-linear programming problem; minimize $f(\mathbf{x})$, where \mathbf{x} is n vector subject to p inequality constrained. And let us say you have a equality constraints, idea is you have a general non-linear programming problem, where you have decision variable, n number of decision variables and several inequality and equality constraints.

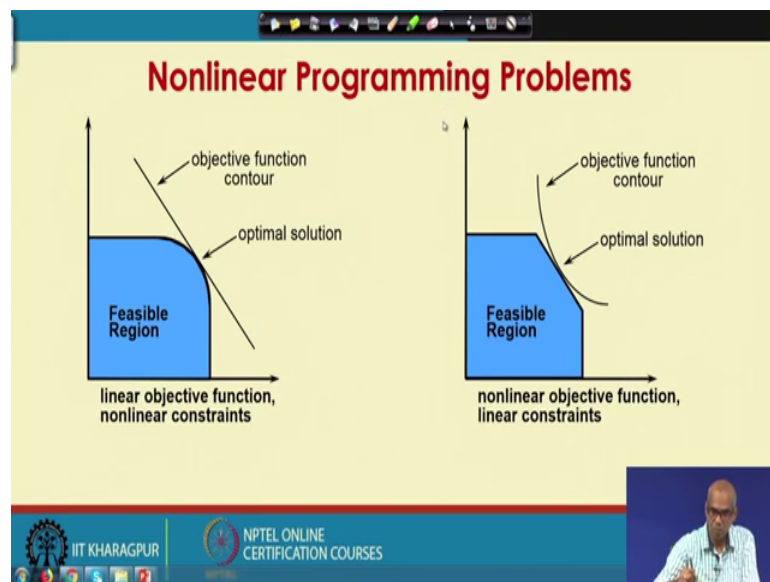
So, first you formulate the Lagrangian. So, to formulate the Lagrangian, we multiply the equality and the inequality constraints with their corresponding multipliers and add them up with the objective function. So, once you have the Lagrangian, the first KKT condition you write that the gradient of the Lagrangian will be equal to 0. Second feasibility check; that means, the inequality constrained has to be satisfied, equality constrained has to be satisfied. So, the candidate solution or candidate optimal solution will satisfy the inequality constrained as well as equality constraints, \mathbf{x}^* is the candidate optimal solution.

We will let us see that, we call this a KKT point, the point that satisfies the all the conditions are known as KKT points. Third KKT condition is switching condition, which says that the product of multiplier of the inequality constraints and inequality constrained will be equal to 0. The non negativity of Lagrange multipliers for inequality constraints

and finally, the regularity check which says the gradients of active constraints must be linearly independent. So, these are the KKT conditions for a general non-linear programming problem. The points that satisfy all these KKT conditions are known as KKT point.

So, a KKT point is the likely candidate for optimum. Remember, the KKT conditions are first order conditions for optimality. So, the KKT conditions are satisfied by the KKT point and the KKT points are likely candidates for optimum. To further the check, if the KKT point is true optimal or not, we must make use of second order conditions and we have seen those things in our previous lectures.

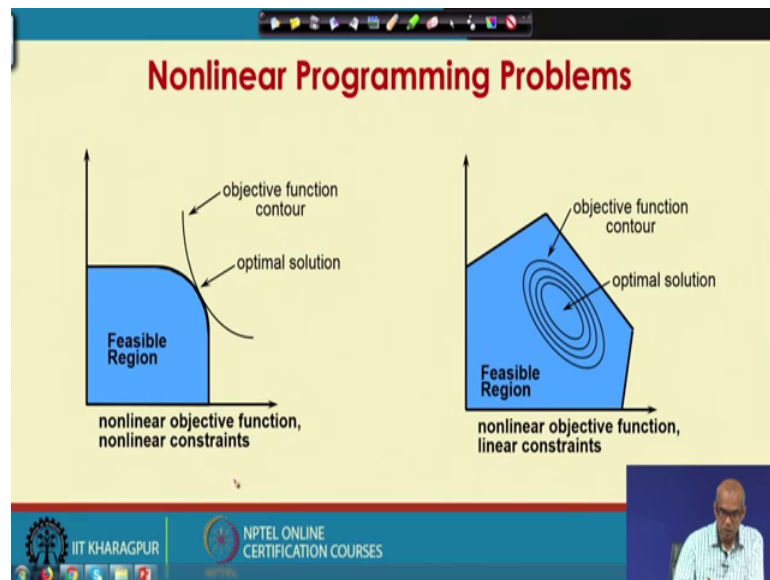
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Now, what you see is a pictorial presentation of a linear objective function and non-linear constraints. And let us say this is the optimal solution.

Here what you see is the constraints are all linear. So, the feasible region is constructed by the linear constraints and the objective function is non-linear. And let us say this is the optimal solution. Look at the difference between the linear programming problem and the non-linear programming problem. Here, the objective function is linear, but the constraints are non-linear and here the constraints are linear, but the objective function is non-linear, but in general non-linear programming problem will have both constraints and the objective function non-linear.

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So, we can have a situation like this, where you have non-linear objective function and non-linear constraints. And the optimal solution is this let us say, but this is not necessary that the optimal solution is always live there. As here, we have a non-linear objective function linear constraints and maybe the optimal solution is lying well within the feasible region.

Note that for linear programming problem, the optimal solution will always be a corner point. So, optimal solution could have been here; in any of this corner points or maybe here, but in case of non-linear programming problem, the optimal solution may lie anywhere within the feasible region.


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Constrained Nonlinear Programming: Techniques

The methods available for the solution of a constrained nonlinear programming problems can be classified into two broad categories: direct methods and indirect methods. Direct methods handle the constraints in an explicit manner. Generally, indirect methods solve the constrained problem as a sequence of unconstrained problems.

<u>Direct Methods</u>	<u>Indirect Methods</u>
<ul style="list-style-type: none">➤ Random search methods➤ Heuristic search methods➤ Sequential linear programming method➤ Sequential quadratic programming method➤ Generalized reduced gradient method	<ul style="list-style-type: none">➤ Transformation of variables technique➤ Sequential unconstrained minimization➤ Penalty function method➤ Augmented Lagrange multiplier method

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Now, let us talk about the techniques or methods that are available for solution of constrained non-linear programming problems. The methods available for the solution of a constrained non-linear programming problem can be classified into two broad categories, direct methods and indirect methods. Direct methods handle the constraints in an explicit manner. Generally, indirect method solves the constrained problem as a sequence of unconstrained problems. Some examples of direct methods were random search methods, heuristic search methods, sequential linear programming methods, sequential quadratic programming method or successive quadratic programming method, generalized reduced gradient method.

Some of the indirect methods are transformation of variable techniques, sequential unconstrained minimization, penalty function method augmented Lagrange multiplier method. So, we will briefly talk about some of these methods in this week.

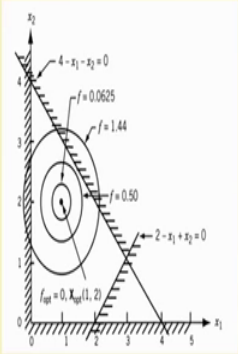
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Characteristics of a Constrained Optimization Problem

1. No effect of constraints:

The constraint may have no effect on the optimum point. In this case, the constrained optimum is the same as the unconstrained optimum.

The minimum point X^* can be found by using the necessary and sufficient conditions.

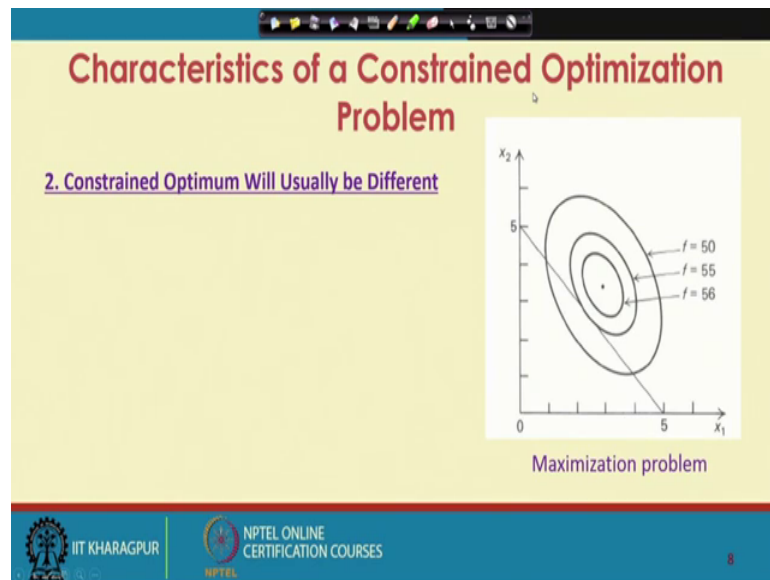
$$\nabla f(X^*) = 0$$
$$\nabla^2 f(X^*) = \text{Positive definite}$$


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Let us look at some characteristics of a constrained optimization problem. It may happen that the constrained has no effect on the optimal solution. In other words the unconstrained optimum and the constrained optimum are the same. This is what you see on the diagram.

Note that the feasible region is such that the constrained optimum is same as unconstrained optimum. In this case the minimum point x^* can be found out by using the necessary and sufficient conditions. For unconstrained minimization there is gradient at x^* equal to 0 and the hessian at x^* is positive definite.

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So, that x^* is a minimum point, but the constraints when they are present will usually have a different optimum than the unconstrained case. Look at the diagram shown; let us say you are solving a maximization problem.

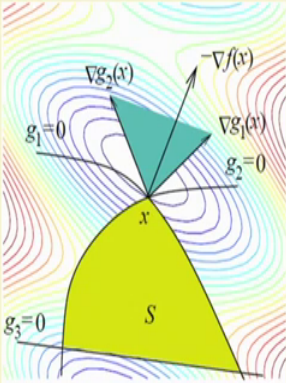
So, this point is the maximum point, you can see from the contours that you see approach this point, the function value increases from 50 to 55 to 56 so, on and so forth. So, now if this is my feasible region, my constrained maximum will be this point, because note that this contour represents a higher function value than this contour; so, constrained optimal will usually be different, but not necessarily.

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Characteristics of a Constrained Optimization Problem

3. Optimum Occurs on Constraint Boundary

According to the Karush – Kuhn – Tucker necessary conditions, the negative of the gradient can be expressed as a positive linear combination of the gradients of the active constraints.

$$-\nabla f(\mathbf{x}^*) = \sum_{j=1}^m v_j^* \nabla h(\mathbf{x}^*) + \sum_{j=1}^p u_j^* \nabla g(\mathbf{x}^*)$$


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So, optimum may occur at constrained boundary. And we have seen when we talked about necessary conditions in our previous weeks, the recording to KKT conditions the negative of the gradient can be expressed as a positive linear combination of the gradients of the active constraints. So, this is what happens when optimum occurs at constrained boundary. Look at the diagram, the active constraints are g_1 and g_2 , g_3 is inactive, point X is optimal. So, the negative of the gradient of the objective function can be expressed as a positive linear combination of the gradients of the active constraints g_1 and g_2 .

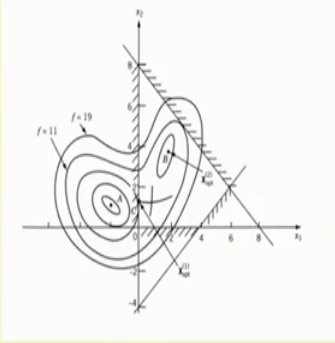
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Characteristics of a Constrained Optimization Problem

4. Multiple Optima

If the objective function has multiple unconstrained local minima, the constrained problem may also have multiple minima.

Sometimes, even if the objective function has a single unconstrained minimum, the constraints may introduce additional local minima.



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A constrained optimum problem, a constrained optimization problem can have multiple optimal solutions. If the objective function has multiple unconstrained local minima, the constrained problem may also have multiple minima. Sometimes, even if the objective function has a single unconstrained minimum the constraints may introduce additional local minima; that means, your unconstrained objective function may have a single minimum, but the constrained objective function may have multiple minima.

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Sequential Linear Programming Method

- The original nonlinear programming problem is solved by solving a series of LPP.
- Each LPP is obtained by approximating the nonlinear objective and constraint functions using first-order Taylor series expansions about the current estimate of the optimum (decision/design variable vector) X_i .
- The LPP can be solved by simplex method to find the new design vector X_{i+1} .
- If X_{i+1} is not the desired (converged) solution, the problem is relinearized about the point X_{i+1} and the procedure is repeated until we find the optimum solution X^* .



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So, now, let us see how we can solve a general non-linear programming problem using successive or sequential linear programming method. So, what are the basic steps? The original non-linear programming problem is solved by solving a series of linear programming problems. Each linear programming problem is obtained by approximating the non-linear objective and constrained functions using first order Taylor series expansion about the current estimate of the optimum; that means, about the current estimate of the decision variable or design variable vector.

The linear programming problem can be solved by say simplex method to find the new decision variable vector. If the new estimate of the solution is not the desired or the converse solution, the problem is re initialized, re-linearized about the point, about the new estimate and the procedure is repeated until you find the optimal solution x^* , so, the method is as follows.

We will solve the linear programming problem by solving a series of linear programming problems. So, first think that you ask is how do I get this linear programming problem from a general non-linear programming (Refer Time: 18:10)

So, what we do is, each linear programming problem is obtained by approximating the non-linear objective function and the non-linear constrained functions using first order Taylor series expansion. And we perform the first order Taylor series expansion around the current estimate of the optimum, let us say the current estimate is X_i .

So, perform Taylor series expansion of the objective function as well as constrained functions around X_i . So, then you will have a linear programming problem, this linear programming problem can be solved by simplex method. And you will get a solution which is an improved estimate of the original non-linear programming problem. Let us say that estimate is X_{i+1} . Now, if this X_{i+1} is the desired solution or the converse solution, we stop. If not, we relinearize; that means, we will linearize the non-linear programming problem again around this new estimate X_{i+1} and repeat the procedure. So, you continue to do this until we converge to the optimal solution or we are very close to the optimal solution.

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Sequential Linear Programming: Linearly Constrained Nonlinear Program

Consider the linearly constrained NLP: This differs from standard LPP only in the presence of nonlinear objective function $f(x)$.

Minimize $f(x)$

Subject to $Ax \leq b$ Now the optimal solution can lie anywhere within the feasible region –
 $x \geq 0$ not necessarily on the corner points only.

The linearization of the above problem around some feasible point x^0 is clearly an LPP and it will have an optimal solution at a feasible corner point, if the feasible region is bounded.

Minimize $\tilde{f}(\bar{x}; x^0)$ How the solution of the approximate problem is related to the
 Subject to $Ax \leq b$ solution of the original problem? Some type of line search is
 $x \geq 0$ required in order to approach the solution of the original
 problem from the approximate solution.

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So, now let us first take the case of linearly constrained non-linear programming problem. So, first we consider the case where the non-linear programming problem have only linearly constrained functions as constraints, so, constraints are all linear. So, we can write it as minimize effect subject to A less or equal to b and we also have non negativity restrictions on x . Note that this differs from standard linear programming problem only in the presence of non-linear objective function $f x$.

So, if the objective function $f x$ will be linear, this will be same as the linear programming problem that we have seen in previous lectures, but a linearly constrained non-linear programming problem differs from standard linear programming problem only in the presence of non-linear objective function. So, now, the optimal solution can lie anywhere within the feasible region, not necessarily on the corner points only.

For a linear programming problem, the optimal solution will always lie, always lie on the corner points, but for a non-linear programming problem the optimal solution can lie anywhere within the feasible region including the corner points. The linearization of the linearly constrained non-linear programming problem around some feasible point x^0 is clearly a non-linear programming problem. And it will have an optimal solution at a feasible corner point provided the feasible region is bounded. So, this I have as linearly constrained non-linear programming problem. So, I linearize this problem around some feasible point x^0 and we obtain this linear programming problem, because now I have objective function linear and the constrained was already linear.

So, this linear programming problem has a solution on any corner point, of course, we are assuming that the feasible region is bounded, but how this solution of the approximate problem; that means, the linearized problem is related to the solution of the original problem. The solution of the approximate problem or the linearized problem will always lie on the corner points, but the solution of the original problem may lie anywhere within the feasible region. So, some type of line search is required in order to approach the solution of the original problem from the approximate solution.

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Sequential Linear Programming: Linearly Constrained NLP: Frank-Wolfe Algorithm

Step-1: Define starting point $x^{(0)}$; Termination parameters $\epsilon > 0, \delta > 0$
 Compute $\nabla f(x^{(l)})$. If $\|\nabla f(x^{(l)})\| \leq \epsilon$, Stop, Else go to Step-2

Step-2: Solve LP subproblem: Minimize $\nabla f(x^{(l)})y$, Subject to $Ay \leq b, y \geq 0$
 Let $y^{(l)}$ be the optimal solution to the LPP.

Step-3: Find $\alpha^{(l)}$ which solves: Minimize $f(x^{(l)} + \alpha(y^{(l)} - x^{(l)}))$, $0 \leq \alpha \leq 1$

Step-4: Calculate: $x^{(l+1)} = x^{(l)} + \alpha^{(l)}(y^{(l)} - x^{(l)})$

Step-5: Convergence check: If $\|x^{(l+1)} - x^{(l)}\| < \delta \|x^{(l+1)}\|$ and if $\|f(x^{(l+1)}) - x^{(l)}\| \leq \epsilon \|f(x^{(l+1)})\|$
 then Stop, Else go to Step-1.

So, we have this algorithm called Frank Wolfe Algorithm which can solve the linearly constrained non-linear programming problem using sequential or successive linear programming. So, in the step 1, we define the starting point and then we define two termination parameters epsilon and delta which are small positive numbers. The current estimate is used to find out the gradient.

So, find out the gradient at the current estimate, if this value is very small we stop otherwise you go to the step number 2. In the step number 2, you solve a linear programming problem which is defined as shown. So, let Y be the solution, optimal solution to the LPP, y t. So, then we do some line search, find alpha which minimizes f of x t plus alpha into y minus x where alpha a number between 0 to 1. So, then we get the estimate of next x t which is x t plus 1 as x t plus 1 equal to x t plus alpha t into y t minus x t f.

The difference between x^{t+1} and x^t is very small or that function value at x^{t+1} minus x^t can be written as less than epsilon into function value x^{t+1} mod of that, we will stop. So, in check this convergence using both the termination parameters. See, if the convergence take is satisfied you stop otherwise we again go to step 1.

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Sequential Linear Programming: General NLP

Consider the following NLP:

Minimize $f(x)$
 Subject to: $g_j(x) \geq 0, \quad j = 1, \dots, J$
 $h_k(x) = 0, \quad k = 1, \dots, K$
 $x_i^{LB} \leq x_i \leq x_i^{UB}, \quad i = 1, \dots, N$

Given an estimate $x^{(t)}$, the following linear approximation problem can be constructed at $x^{(t)}$.

Minimize $f(x^{(t)}) + \nabla f(x^{(t)})(x - x^{(t)})$
 Subject to: $g_j(x^{(t)}) + \nabla g_j(x^{(t)})(x - x^{(t)}) \geq 0, \quad j = 1, \dots, J$
 $h_k(x^{(t)}) + \nabla h_k(x^{(t)})(x - x^{(t)}) = 0, \quad k = 1, \dots, K$
 $x_i^{LB} \leq x_i \leq x_i^{UB}, \quad i = 1, \dots, N$

Solution to this LPP gives us $x^{(t+1)}$.
 If $x^{(t+1)}$ is infeasible, reinitialize at $x^{(t+1)}$.

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So, now let us look at the case of general non-linear programming problem, how a general non-linear programming problem can be solved by sequential linear programming method?

So, let us considered a general NLP as shown, minimize $f(x)$ subject to $g_j(x) \geq 0, j = 1$ to $J, h_k(x) = 0, k = 1$ to K and x is bounded between lower bound and upper bound solution to this linear programming problem,. So, given, given an estimate x^t , we can linearize this given non-linear programming problem by Taylor series expansion, we written only the first order terms and can get this set of expressions or this linearized problem. Note that $f(x)$ has been linearized around x^t as $f(x^t) + \text{gradient of } f \text{ evaluated } x^t \text{ into } x - x^t$. Similarly, the inequality constrained has been approximated using Taylor series expansion.

Also the equality constrained has been approximated by performing Taylor series expansion and retaining first order tern. So, solution to this linearized problem or linear programming problem gives us x^{t+1} solution, if x^{t+1} is in feasible, we will re linearize the original problem at x^{t+1} and this will continue until we converge

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Sequential Linear Programming: General NLP: Example

Consider the following NLP:

Minimize $f(x) = x_1^2 + x_2^2$ $\nabla f = \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix} = \begin{bmatrix} 4 \\ 2 \end{bmatrix}, f(2,1) = 5$ $\nabla g = \begin{bmatrix} 2x_1 \\ -1 \end{bmatrix} = \begin{bmatrix} 4 \\ -1 \end{bmatrix}, g(2,1) = 3$

Subject to: $g(x) = x_1^2 - x_2 \geq 0$ Now, $f(x^{(t)}) + \nabla f(x^{(t)})(x - x^{(t)})$ Now, $g(x^{(t)}) + \nabla g(x^{(t)})(x - x^{(t)})$



$h(x) = 2 - x_1 - x_2^2 = 0$ $= 5 + \begin{bmatrix} 4 & 2 \end{bmatrix} \begin{bmatrix} x_1 - 2 \\ x_2 - 1 \end{bmatrix}$ $= 3 + \begin{bmatrix} 4 & -1 \end{bmatrix} \begin{bmatrix} x_1 - 2 \\ x_2 - 1 \end{bmatrix}$

$0.5 \leq x_1 \leq 2.5, 0 \leq x_2 \leq 3$ $= 5 + 4(x_1 - 2) + 2(x_2 - 1)$ $= 3 + 4(x_1 - 2) - (x_2 - 1)$

We want to construct the linear approximation to this problem at $x^0 = (2, 1)$.

$\nabla h = \begin{bmatrix} -1 \\ -2x_2 \end{bmatrix} = \begin{bmatrix} -1 \\ -2 \end{bmatrix}, h(2,1) = -1$

Now, $h(x^{(t)}) + \nabla h(x^{(t)})(x - x^{(t)}) = -1 + \begin{bmatrix} -1 & -2 \end{bmatrix} \begin{bmatrix} x_1 - 2 \\ x_2 - 1 \end{bmatrix} = -1 - (x_1 - 2) - 2(x_2 - 1)$

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So, let us take an example minimize $f(x)$ equal to x_1 square plus x_2 square, subject to x_1 square minus x_2 greater equal to 0, 2 minus x_1 minus x_2 square equal to 0. And x_1 has upper bound as 2.5 and lower bound as 0.5. Similarly, x_2 is constrained between 0 and 3.

So, on to constrained the linear approximation to this problem at x^0 equal to 2, 1, so, 2, 1 is the current estimate. So, let us find out the gradient of the objective function, we found it out as $2x_1$ and $2x_2$, evaluate it at point 2, 1. So, you get 4, 2 the function value at point 2,1 is 5. So, now, the objective function is approximated by performing Taylor series expansion and we get this. So, this is f of x t, this is the gradient and this is x minus x t greater.

So, now let us do the same for the inequality constrained and you get this as the linearized in equality constrained. And also let us do the same thing for equality constrained and we get this as a the linearized equality constrained.

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Sequential Linear Programming: General NLP: Example

Consider the following NLP:

Minimize $f(x) = x_1^2 + x_2^2$
Subject to: $g(x) = x_1^2 - x_2 \geq 0$
 $h(x) = 2 - x_1 - x_2^2 = 0$
 $0.5 \leq x_1 \leq 2.5, 0 \leq x_2 \leq 3$

Minimize $f(\bar{x}; x^0) = 5 + 4(x_1 - 2) + 2(x_2 - 1)$
Subject to: $\bar{g}(\bar{x}; x^0) = 3 + 4(x_1 - 2) - (x_2 - 1)$
 $\bar{h}(\bar{x}; x^0) = -1 - (x_1 - 2) - 2(x_2 - 1)$
 $0.5 \leq x_1 \leq 2.5, 0 \leq x_2 \leq 3$

The solution to this LPP is $x^{(1)} = (11/9, 8/9)$
 $g(x^{(1)}) = 0.6049 > 0, h(x^{(1)}) = -0.0123 \neq 0$

Therefore, we reinitialize the problem at $x^{(1)}$.

Continue until we get $x^* = (1, 1)$ as optimal solution.

So, when you put all this things together, we get this linearized problem for the original non-linear programming problem. This linearized problem or the linear L, linear programming problem has a solution 11 by 9 as x_1 and 8 by 9 as x_2 . Let us check, if the inequality constrained and the equality constrained are satisfied in equality constrained is satisfied.

But equality constraint is not satisfied is minus 0.0123, if it is very - very small, we will take it as 0, but we can do better. So, therefore, we will reinitialize the problem; that means, we will re linearize the problem at x_1 which is 11 9 and 8 by 9 and we will proceed as follows. So, basically what will do is we will make use of this, this and this, but the points now will be x_1 that is that 11 by 9 and 8 by 9

So, that will give you x_2 , we will continue to do this until we are very close to the true optimal solution and the optimal solution, true optimal solution is 1, 1. If you look at here, we are not very very far from 1, 1 is the rough approximation of 1, 1, but if we take 2, 3 iterations more just repeating the same steps, you will see that we are getting very close to the true optimal point 1, 1. So, this is how we can solve a general non-linear programming problem using successive linear programming methods. So, with this we stop lecture 46 here.