Computational Techniques

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Module No.# 04

Lecture No. # 05

Nonlinear Algebraic Equations

Algebraic equations the equations of the type f x equal to 0. So we want to find the values of x that are going to satisfy the equation f x equal to 0. We have looked at several methods bracketing methods and open methods to solve the problem of f x equal to 0. And of these methods that we have looked at, we have specifically considered the fixed point iteration the Newton-Raphson method, and the bisection method to see look at there stability and convergence properties.

That is what we have essentially done. So far we have specifically focused on problems in single variable what is actually going to be also important is look at problems in multi variables.

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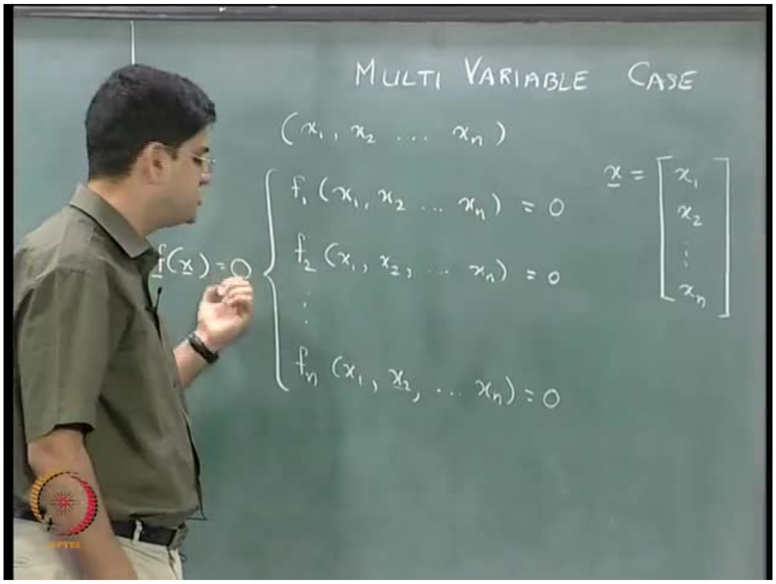

Just to motivate the problem in multi variable this is what we have we had looked at. When in the first lecture of that module of this module so extension to multi variables. So let say we have instead of a single variable x we have n variables x 1, x 2 and so on up to x n and these variables satisfy set of equations which is f 1 of x 1, x 2 and so on up to x n equal to 0 f 2 of x 1, x 2 up to x n equal to 0 and so on until f n of x 1, x 2 up to x n equal to 0.

These are the n equations in n unknowns and the short hand notation for writing all this is f bar of x bar equal to 0 bar. So often times we will just write this as f of x equal to 0 and based on the context we will figure out that this is actually a single variable or a multi variable case but, what x bar means is nothing but, x 1 at x 2 up to x n just the same notation that we had used earlier in our linear systems part.

So, f bar x bar is nothing but, x 1 x 2 up to x n and f bar is nothing but, f 1 as the first element f 2 as the second element and so on up to f n as the nth element in in this particular equation. So, what we are interested in doing is to extend the numerical methods that we have talked about two problems of of this sort of trying to get x 1 up to x n which are solutions to f of x bar equal to 0.

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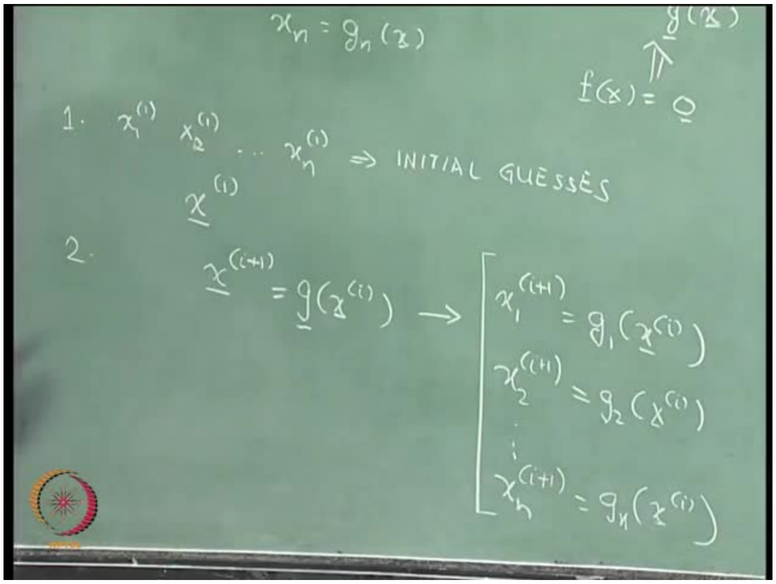

That is our aim in in today's lecture and two methods that we are going to look at is the fixed point iteration and the Newton- Raphson method. So let us look at the extension extension of fixed point iteration method and the extension of fixed point iteration in this case what we are going to write write the equations. we are going to write the equations in the form of x 1 bar x 1 of x 1 is going to be equal to g 1 of x bar x 2 equal to g 2 of x bar and so on up to x n equal to g n of x bar.

And as we had seen in in one of the previous lectures what what how we can convert f of x equal to 0. In this form there is not there isn't a unique way in order to convert f of x into into this form one very straight forward and not necessarily the best way but, one straight forward way of writing g bar is we can write the equation to the equation f of x bar equal to 0 we can add x bar on either sides and we can write x bar is going to be equal to x bar plus f bar of x bar and this we can call as our g of g bar of x bar.

This is one straight forward or simple or new way of converting f x equal to 0 to convert f f x equal to 0 to the form x equal to g of x. so, this is one straight forward way of doing this and once once we do this we will essentially get x 1 equal to g 1 x 2 equal to g 2 and so on up to x n equal to g n. This is what we are going to get and let us recall what we did essentially in Jacobi iterations and that is that is pretty much what we are going to do in fixed point iteration in multiple variables. What we will do is let us say we so we will start off with initial guess x 1 1 x 2 1 and so on up to x n 1. These are going to be our initial guesses which we can in a short hand notation we can write write this down as nothing but, x bar of 1.

We will start off with the initial guesses x 1 1 x 2 1 up to x n 1 and then we will use the fixed point iteration in order to get i plus oneth value from given the ith value, And the short hand notation it is a very straight forward way of writing in in short hand notation and that is going to be x bar of i plus 1 is going to be equal to g of x bar I. what this essentially means is its it essentially means is x 1 i plus 1 is going to be equal to g 1 of x i x 2 i plus 1 is going to be equal to g 2 and so on up to x n i plus 1 equal tog n of x I, And this is what we we really mean by by this particular expression.

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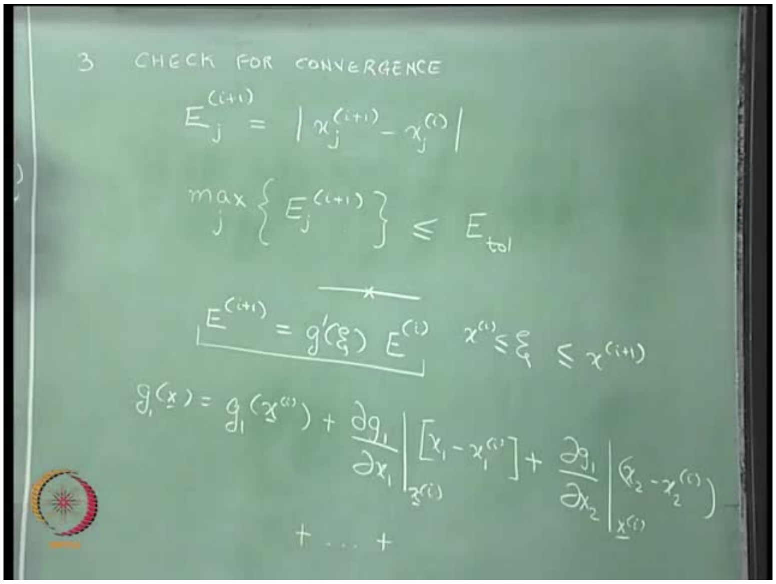

Now the question is when do we stop and when do we say that the particular equations have converged so, the third sign the third item in our algorithm is to check for convergence. And in this particular case we are going to define our error E i we are going to define is a e or rather we should say E i plus 1 keeping in touch with what we were doing in earlier lectures. E i plus 1 is going to be define for each variable it will it will be define for x 1 x 2 and so on up to x n.

In general E i plus 1 j will be defined as the difference x j i plus 1 minus x j i. The absolute value of this this is going to be our E j i plus 1 and the objective is that so for example, we have x 1 x 2 up to x n we want to ensure that the largest among these error values is going to be less than certain tolerance and that is what we are going to write write this down is we will write down maximum over j of E j i plus 1 should be less than or equal to E tolerance. And this is the criterion that we are we are going to going to look at for example, if the true solution in two variables if the true solution is one one and one and let say that x 5.

Let this is the true solution x bar and let say at certain point x 5 turns out to be 1 and 1.05 then the error in this particular case is 0 the error in this particular case is 0.05. And the max when we run max over the errors over here the max value is indeed 0.05, which is not going to be less than our tolerance value of say 10 to the power minus 4. And in if that is the case we are going to keep running these iterations over and over again until we run we reach the desired converge desired convergence levels.

This is what we will we will get so if until these particular condition is satisfied the fixed point iteration are going to be repeated over and over again. Now let us now consider the convergence criterion therefore the fixed point iteration what we had done for with fixed point iteration in the previous lecture is that we we had found that the error E i plus 1 was going to be equal to g dash of zeta multiplied by E i where zeta was some point that lied between x i and x i plus 1. It need not I mean the the science might you will possibly be over as well of x i is greater than x i plus 1 so, zeta is a point that lies between x i and x i plus 1.

This is the expression that we essentially got for a single variable case. And this trick came outright out of the new as excuse me this came right out of writing or expanding the Taylor series expansion and throwing away the terms in the second order and higher orders in in the Taylor series. Keep in mind that the Taylor series expansion in multi variable case is going going to going to be going to look like.

so, g of x bar is going to be equal to g of x i or let let us say g 1 is going to be equal to g 1 of x I plus partial g 1 with partial x 1 computed at x x bar i multiplied by x 1 minus x 1 I, plus partial g 1 with respect to x 2 computed at x computed at x bar i multiplied by x 2 minus x 2 i and so on up to the nth order term. And then we will have the second order second derivative terms and so on, keep in mind that for a single variable this is the same as g dash of of zeta.

If we were to extend this particular error analysis to something in n variables. So, instead of having just g dash of zeta multiplied by E i we will have essentially d g by d x d g by d x 1 plus d g by d x 2 plus d g by d x 3 and so on and so forth. And those are the terms we are going to get just an extension of this particular expression two an nth variable n variables case case and you can look up any of this standard text books such as, the once given in the the overall syllabus for for this particular a lecture series. So, this chapra and canale numerical methods by chapra and canale numerical methods by for engineers by s k gupta or you can look at basically numerical recipes in see by press at all.

Any of these standard books if you go and refer to them some of the derivations for what we are doing more more detail derivations will be provided by them. I am not going to go run through the details but, but essentially what you will get is E i the error at i plus oneth iteration in the jth variable is going to be equal to we will have this gg dash terms for g 1 with for g j with respect to each of the variables.

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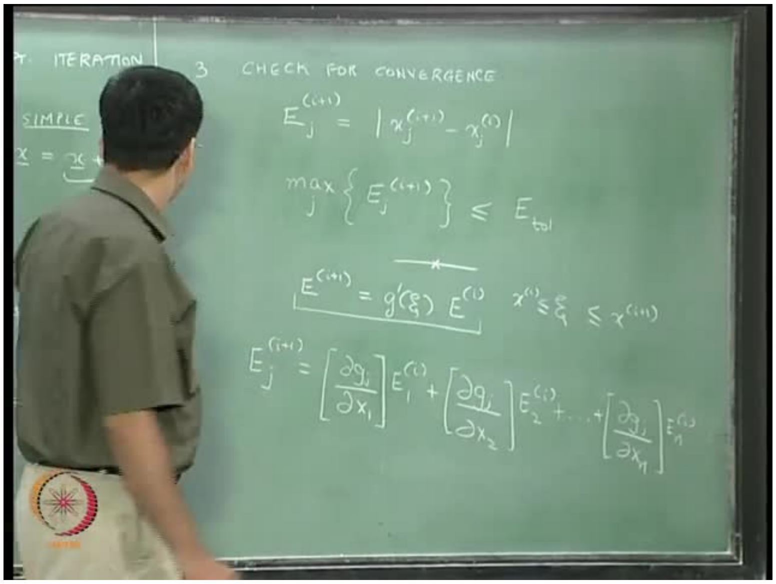

We will have partial g j by partial x 1 multiplied by E i 1 plus partial g j by partial x 2 multiplied by E i 2 and so, on to partial g j divide partial by partial x n multiplied by E i n.

This is the error in the i plus oneth iteration for the jth variable. And what we we need to do essentially is to find out the maximum of of those errors and see how that maximum error compares to epsilon tolerance and without actually getting the going through the derivation what I will write is, I will write the final results for that will guarantee the tolerance and the final result some of you might might immediately be able to see the final result with respect to a single variable case was just g d g by d x was the absolute value of that would be less than one that was the sufficient conditions to guarantee stability. Now the sufficient condition to guarantee stability is going to be sum of all these guys the sum of all these should be less than or equal to 1.

I will write down the condition for stability.

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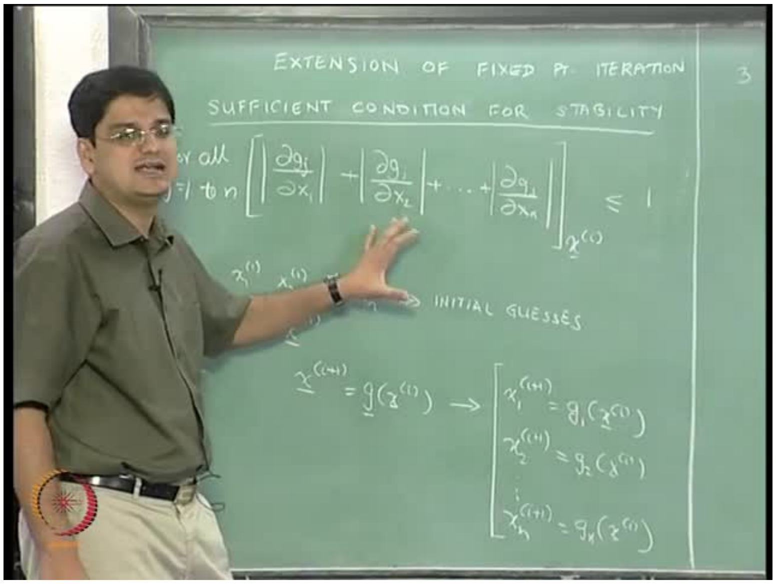

For the the fixed for the fixed point iteration the sufficient condition for stability is going to be d g d g d j by d x 1 plus d g j by d x 2 and so, on up to d g j by d x n computed at x bar of i should be less than or equal to 1.

For all j equal to 1 to n. So, what that means is partial g 1 by partial x 1 plus partial g 1 by partial x 2 and so, on up to partial g n by partial g 1 by partial x n that should be less than one and the same would be true for partial g 2 by x 1 g 2 g 2 by x 2 plus g 2 by x n that also should be less than one and up to for all the n functions.

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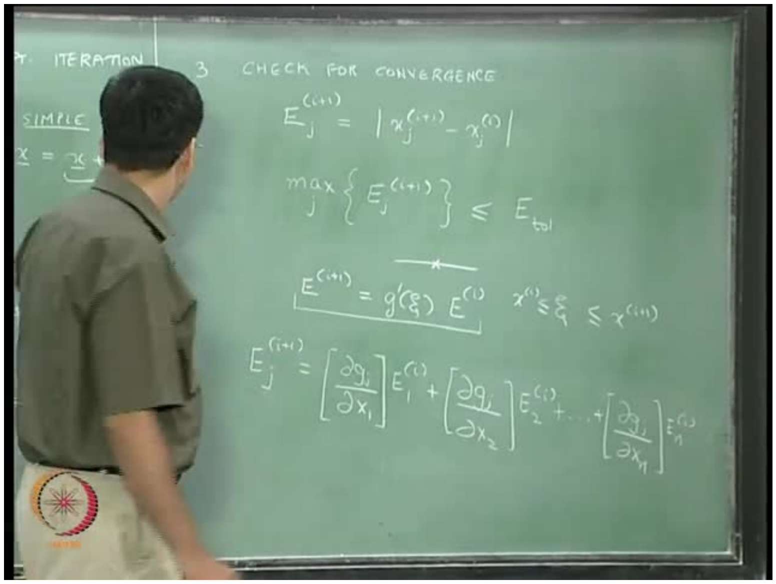

That is essentially the the sufficient conditions for sufficient condition for stability of the fixed point iteration. Now one of the comments about this particular sufficient conditions for stability of fixed point iteration is this is, this is a fairly stringent condition for a general function a general set of functions g i to be met and it is not always possible in a general non-linear set of equations for this conditions to be met that actually is something that will limit the applicability of the fixed point iteration. The first problem is at the overall fixed point iteration method is linearly convergent as we have seen over here is that the error E i plus 1 depend is proportional to error E i to the power 1. It is a linearly convergence system and it remains linearly convergent when you have essentially multiple variable case also the overall convergence of of this a system is not guaranteed for large number of problems of are of are interest. One of the things that we had done earlier in order to convert a general expression to the form f of x bar was if when we are to to the form x equal to g of x.

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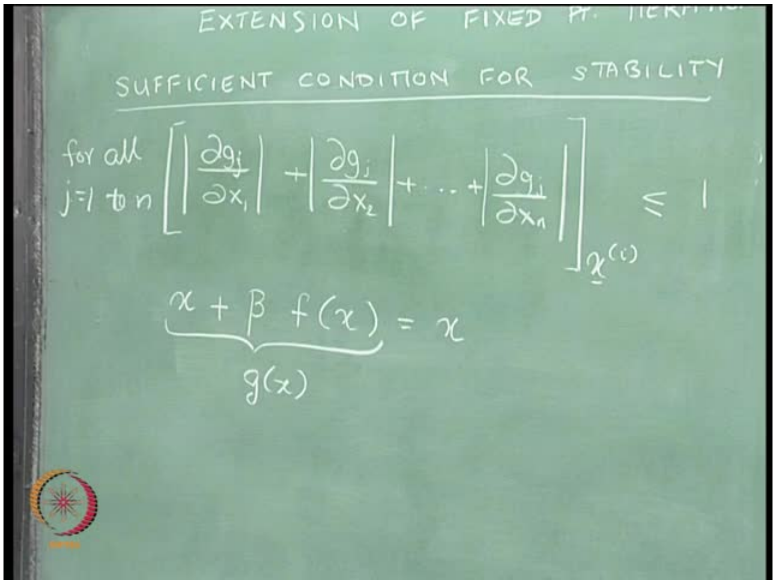

Let us say we started with f of x equal to 0. What we what we had done essentially in this in this particular case is we, had added x bar on on to the either to on to either side of this equation.

We can actually do a slight modification to that if f of x equal to 0 is the problem that we want to solve, we can multiply this equation by beta. If f of x if if the solution for f of x equal to 0 we need the solution for beta multiplied by f of x equal to 0 is also going to be the same solution and then on both sides we can add plus x.

What we will get essentially is an equation of this particular form and this becomes our g. So, x equal to x plus beta time's f of x is going to be our g and we can then judiciously select our beta such that this sufficient condition for convergence is satisfied. It is possible to do that sometimes the beta that you will need is going to be a very small value beta and if if that is the case the the moves that will be made by a a fixed point iteration method are going to be very conservative moves that means we are going to move very slowly towards the solution. When we have this as our our g of x what we will get is g dash of x is going to be nothing but, one plus beta times f dash of x.

We want our f dash of x to be negative in order for for this to work. if if f dash of x is going to be positive we can take a negative value of beta. So, we can appropriately choose that value of beta such that the sufficiency of this of of the condition d g by d x less than or equal to 0 is satisfied not that fixed point iterations or not applicable is just that the applicability range of the fixed point iteration method often in practical chemical engineering problems at least in my experience has been fairly limit.

That is about the fixed point iteration. We now go on to the work horse which is essentially the Newton- Raphson method and we will we will look at extension of Newton- Raphson's method to a multi variable case.

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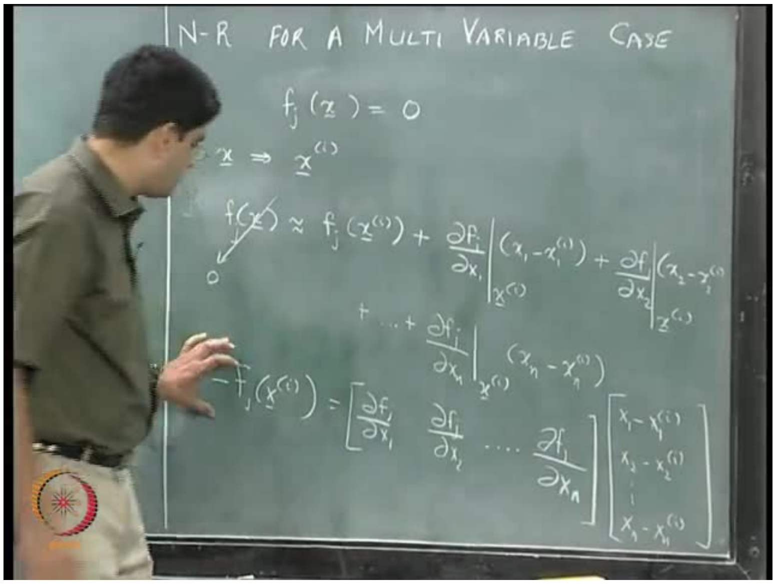

Now we are going to look at the Newton- Raphson's method for for a multi variable case. So, we have f 1 of x bar equal to 0 f 2 of x bar equal to 0 and so on.

Let us consider any jth function f j of x bar equal to 0. And so and currently we have the the guess the current guess of x bar current guess is x bar at i. So, what we are going to do is we are going to line arise f j of x bar around x bar i and that we can write down and as f j of x bar is going to be approximately equal to f j of x bar i , plus we will have d f j by d x 1 multiplied by x 1 minus x 1 i plus d f j by d x 2 multiplied by x 2 minus x 2 i. And this is evaluated at x bar i and so on up to d f j by d x n evaluated at x bar of i multiplied by x n ith iteration multiplied by x n minus x n at ith iteration plus higher order terms.

This is what we get if we neglect the higher order terms we will get this particular expression as approximately equal to the right hand side. Now, what we had done in deriving the Newton-Raphson's method is we we had put this particular guy equal to 0 and whatever solution that we get was x of i plus 1 that is what we had we had done.

This is essentially this amounts to looking at keeping only the linear terms in the expression. when when We essentially do that we will take so, we will we have put this guy equal to 0 will take the f j on to to the left hand side and when we do that we can in the matrix notation we will be able to write this particular equation as negative of f j computed at the ith value is going to be equal to d f j by d x 1, d f j by d x 2 and so on up to d f j by d x n. These are all evaluated at x bar I, the ith value ith guessed value of x bar multiplied by x 1 minus x 1 i x 2 minus x 2 i and so on up to x n minus x n i.

This is what we are going to get for f j. we will will get this for f 1 we will get this for f 2 we will get this for f 3 and so on we will get this for all of the n n functions. So, we what we can do is then we stack this particular things together what we will get.

To simplify this a little bit what I will do is I will just go go over for a two variable case so, just f 1 and f 2 and then we can we can see what happens in two variable case and we will able to extended to n variable case.

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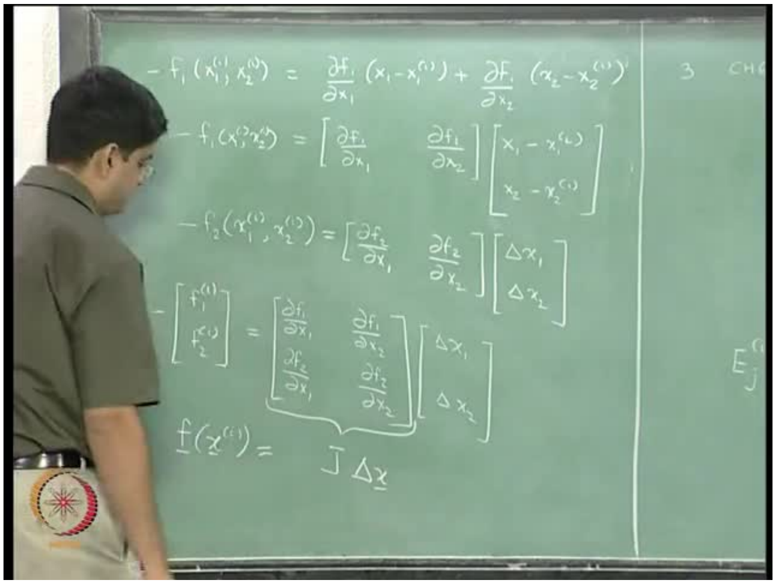

In the two variable case, we will have f 1 of x 1 comma x 2 is going to be equal to dou f 1 by dou x 1 x 1 minus x 1 i plus dou f 1 by dou x 2 x 2 minus x 2 i. And this we can also write it as dou f 1 by dou x 1 and dou f 2 by dou f 1 by dou x 2 this multiplied by x 1 minus x 1 i and x 2 minus x 2 i.

That is going to be minus f 1 of x 1 comma x 2 or rather minus f 1 of x 1 i comma x 2 i. I miss the i subscribes over here likewise, we will be able to write this for f 2 as well and for f 2 this will end up being f f 2 computed at x 1 i and x 2 i is going to be equal to partial f 2 by partial x 1 partial f 2 by partial x 2 multiplied by and again, I am just going to be a little bit lazy and use a short hand notation over here and I will call this as d x 1 and d x 2.

These are going to be two equations which we can then combined together to write this as minus f 1 and f 2. And again I am being lazy and writing the short hand notation over here this going to be equal to partial f 1 by partial x 1 partial f 1 by partial x 2, these two guys will be upon the first row and on the second row we will have partial f 2 by partial x 1 and partial f 2 by partial x 2 multiplied by delta x 1 and delta x 2 multiplied by value of delta x 1 and delta x 2 that solve these equation linear equation are nothing but, the difference between the i plus 1 th value of x and ith value of x.

We will invert this particular matrix. So, we will represent this as j multiplied by delta x bar is going to be equal to f bar computed at x bar i. So, our delta x is going to be nothing but, j inverse f that is going to be what our our delta x is so, our delta x bar is going to be equal to minus j computed at x bar of i inverse multiplied by f bar computed at x bar of i .This is this is essentially what what we will we will get if I look at if I go back to an expression over here I made slight error in this I missed out the negative sign over here. This negative sign has to be there what we have done is inverse take to taken j inverse multiplied it over here and if you notice this this is essentially equivalent to the problem that we had solved in module three the problem was b equal a x and we wanted to find the solution to the linear equation b equal to a x.

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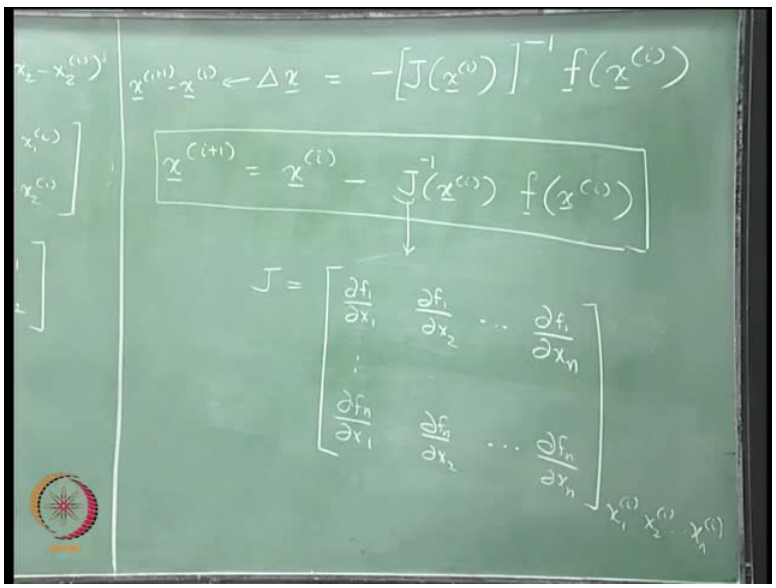

In order to find this delta x bar you can use any of those methods such as gauss elimination or gauss sidle method or any of those method in order to get delta x bar equal to negative of j inverse multiplied by f. And remember the delta x what we had was nothing but, x i plus 1 minus x bar at i. Again these are vectorial notations which basically means it does matter whether you pre multiply or post multiply j this is a pre multiplication by j inverse.

What we will get eventually is x bar of i plus 1 is going to be nothing but, x bar of i minus j inverse computed at x bar of i multiplied by f bar computed at x bar of i. For n n by n system j inverse or j is going to be nothing but, partial f 1 by partial x 1, partial f 1 by partial x 2, and so on up to partial f 1 by partial x n. Like the second role we partial f 2 by partial x 1 partial f 2 by partial x 2 and so, on up to partial f 1 f 2 by partial x n and we will continue that to partial f n by partial x 1 partial f n by partial x 2 up to partial f n by partial x n this computed at x 1 i x 2 I and so on up to x n i.

This is going to be our matrix j our f is nothing but, f 1computed at x bar of if two computed at x bar of i so on. And so, forth this is going to be our multi variable Newton- Raphson's equation. Again to recap we have d f 1, d f 1, d f 1 on the first row d f 2, d f 2, d f 2 on the second row and so, on up to d f n, d f n, d f n on on on the nth row of the Jacobian matrix.

That is the essentially what we get with respect to the Newton- Raphson's method the convergence the order of convergence for the Newton- Raphson's method is going to quadratic order. And that is really because what we have done with the Taylor series expansion is that we have retained the the Taylor series up to the first derivative term and we have discarded the second derivative term and the term that is discarded the leading term that gets discarded has an error which which depends on square of that term and that is the reason why a Newton-Raphson's method has a quadratic convergence rate.

This was essentially the extension of fixed point iteration and the Newton-Raphson's Newton-Raphson's method to multi variable systems. So, extension or improvements to Newton-Raphson's method is what I am going to consider next.

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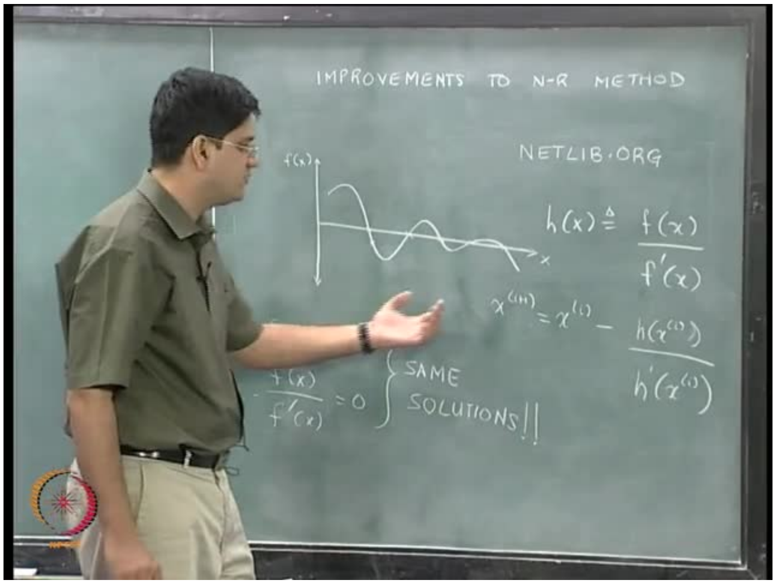

And what we will do is we will start with a single variable case I am not going to go through the derivations. what what I want to want to give you a flavor of is that there are several improvements improvements to the Newton- Raphson's method that we have come up with in the last 8200 years and those improvements to look at those improvements you can go and use various sources and one of very good source is to start off with is a numerical recipes in c or fortran. That is the name of the text book this is text book that you can refer it is a very very good resource for all numerical techniques and it is available on the website n r dot com. So, you can go to the website n r dot com and take a look at the numerical recipes text book. The numerical recipes text book is not free freely available for on the website I believe it is something like 19 dollars or something like that to to download the latest copy of the numerical recipes text book. The earlier versions are the in second addition of numerical recipes text book I believe are available for free for free to download. You can go to n r dot com and download essentially addition second addition and I believe that was numerical recipes and Fortran that is the second addition that is available for download from n r dot com and it is a very good resource if if numerical if you want to understand or use numerical recipes in a better way.

Likewise if you want to just use some of the numerical techniques then there is another website called net lib dot o r g. This is an online repository of a lot of numerical numerical codes that including linear algebra non-linear equation solving o d e solving and so on that is available freely for downloading you can go to net lib dot org and choose on appropriate solver f f o or going to use any kind of complicated problems that you intend to solve. The objective of this particular lectures is to give you an overview of the or an introduction to the numerical numerical methods to computational techniques so, that you can get the confidence to go and look at some of the the more advance methods that that are being being use.

Anyway the the improvements to the Newton- Raphson's method the several ways in which people have figured out how to improve the Newton- Raphson's method. And all of them are for looking for particular set of problems, one of the improvements that was done that was done by Ralston's. Essentially is for let say we have f of x versus x and if we plot say f of x and lets arbitrarily this is the kind of curve that f of x we get where f of x is going to intersects set the x axis at multiple points.

Now we know that Newton- Raphson's method starting from an initial guess which is close enough to the solution converges very quickly to the solution there is second order convergence to any of this solution. However if a Newton- Raphson's method is going to be use in order to find the multiple solutions to this to the equation f x equal to 0 it fairs quite poorly it it does not converge as quickly as as one one one would like.

what what researches figured out in 19 1970'S late 1970's. Essentially is is that we have the the equation x i plus 1 equal to x i minus f i divided by f dash it is a typical Newton- Raphson's method. What we can do a slight modification to this particular method could be to multiply this with some factor m and the question is what what is the factor m that we choose, and ralston's essentially came up with this m should be the number of solutions that you get the number of times that this particular curve intersects the x axis.

In this particular case the m that I am going to use is going to be four in order to get the fourth solution to f x equal to equal to 0. And by using this particular method they found that by by choosing m equal to 1 they will be able to get the first solution very quickly in order to go to the second solution you choose you choose a different value of m in order to improve the convergence rate.

The problem with choosing this m is in general when you are given when when we are given general f of x we do not know a priory how many times this f of x is going to intersects intersect the x axis. And if that information is not known a priory we may not really be able to use m equal to four for example, in in this particular case if we do not know the four roots of this particular equation exits.

That is one one issue with with this particular method but, what the same researches realize is that if the solution to f of x equal to 0 and the solution to f of x divided by f dash of x equal to 0 these two functions have the same solutions.

It can be numerically be prove that the function f of x divided by f dash of x has the same solution as the function f of x a f of x equal to 0.

What this guy did is is instead of using this particular way of solving things they define a new function let us called h of x. They defined h of x has nothing but, is defined as f of f x divided by f dash of x this is going to be our our h of x. And now the objective instead of finding the solution of f of x the objective is now change to find solution of h of x and that is that is becomes new problem.

what what we can have is x of i plus 1 is going to be equal to x of i minus h of x of i divided by h dash of x of i. And this is going to have a for the function h of x this will have the same convergence properties as the Newton- Raphson's method but, in order to get the solution of f of x this will have a faster rate of convergence then the original Newton- Raphson's method which was essentially x i plus 1 equal to x i minus h of x of i.

What we can then do is we can expand this h i prime as nothing but, f prime squared minus f multiplied by f double prime divided by ff prime square, that is what we will get over here and h is nothing but, f divided by f prime and we can rearrange and we can get this this over all expression. And if you are interested in knowing you can look at this particular method in any of this standard standard text text books that follow.

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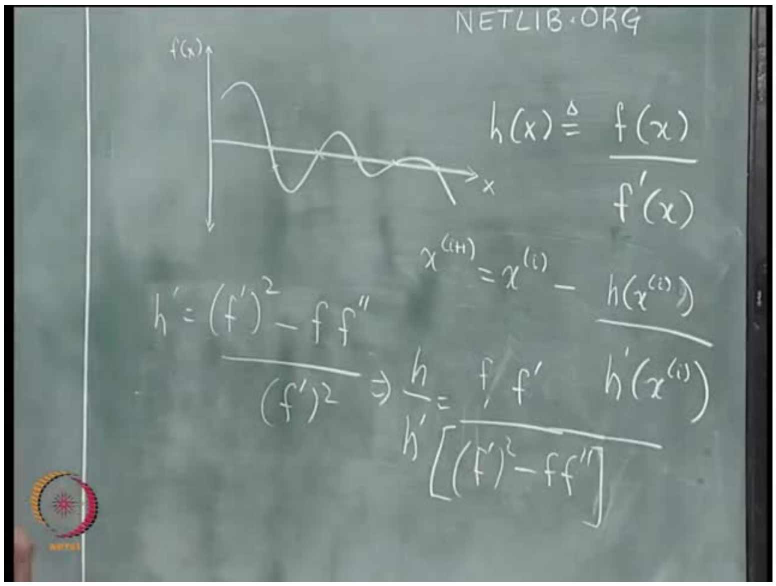

We will we will just look at what what this particular expression by using this would mean our h dash. As I said is going to be f dash multiplied by f dash which is f dash squared minus f multiplied by f double dash divided by f dash squared. This is what our h dash is going to be so, h divided by h dash is so, h by h dash is going to be nothing but, f by f dash divided by f dash squared minus f f double dash and this whole thing divided by f dash squared.

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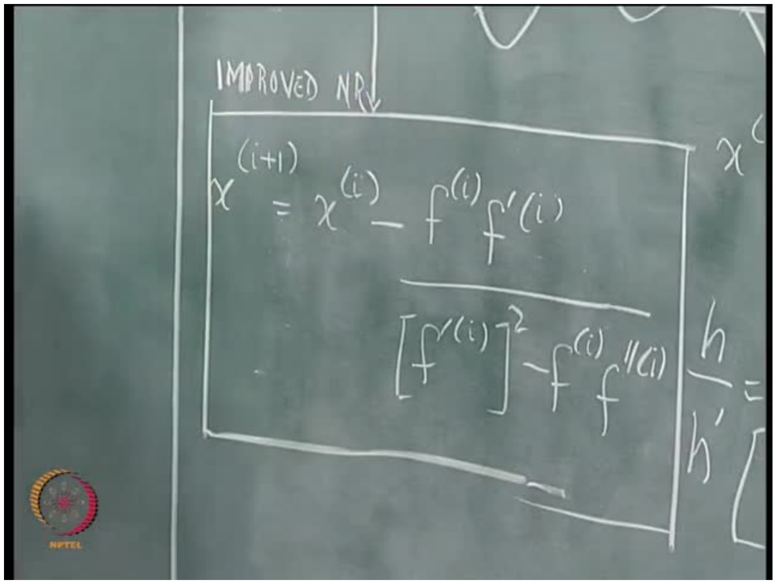

You take f dash squared over here. So, to the numerator and you will get f dash and one of the f dash f dash is will get canceled. This will get canceled along with this and then when you take f dash on to the numerator you will essentially get f f dash. So, this is going to be our h divided by h dash so, using that equation and if you haven't follow the derivation what i i suggest you can you you can do is take a piece of pen pen and paper and read arrive it yourself more slowly but, what we can get is x i plus 1 equal to x i minus f i f prime i divided by f prime i squared minus f i and f double prime i. And this is going to be our improved Newton- Raphson’s method.

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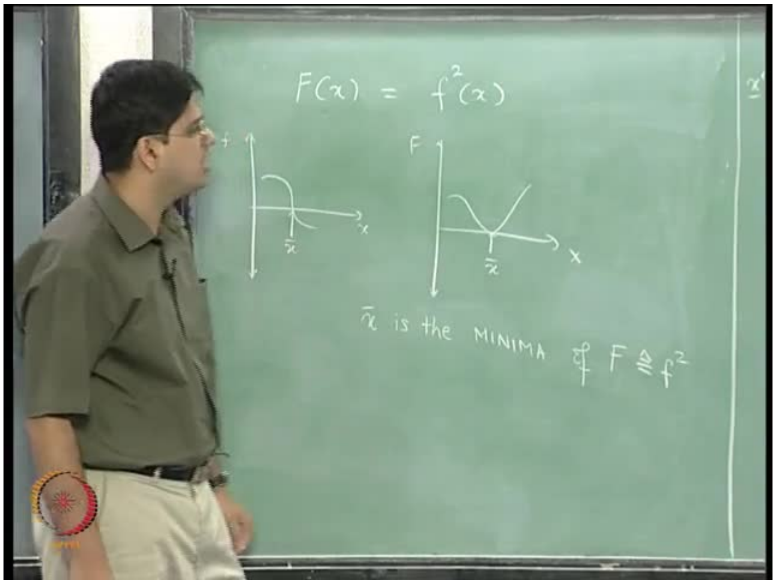

Let us define our function f of x as equal to f square of x. so, we have just squared this particular function. Now f of x because it is just square is going to always be positive except when x is the solution to f of x equal to 0 when f of x go is going to be equal to 0 our f x is going to also be equal to 0, for all other values off of x our capital f x is going to be positive.

For example, for a general function of this this short of this is f versus x our f f versus x is going to be something like this. Where this and this are the same values so, if we all these as the solution x bar this is going to be the same as x bar. Therefore, x bar is the minima x bar is the minima of f which is defined as going to be equal to going to be equal to f square and we can use essentially this property in order to get and improvement in the Newton Newton-Raphson's Newton- Raphson's method. And the improvement Newton- Raphson's method using this particular property has gotten to do with the first and second derivatives of this function function f of x this is little bit more advance for for the sake of our course I am just mentioning it so, that some of you who are interested in learning the Newton- Raphson's method can then go ahead and look at some of the more advanced versions of of the Newton- Raphson's method. And again the place where you can start off with is the numerical recipes by press at all the that book would be a good source to start off with going into more advance topics in the non-linear non-linear equation solving.

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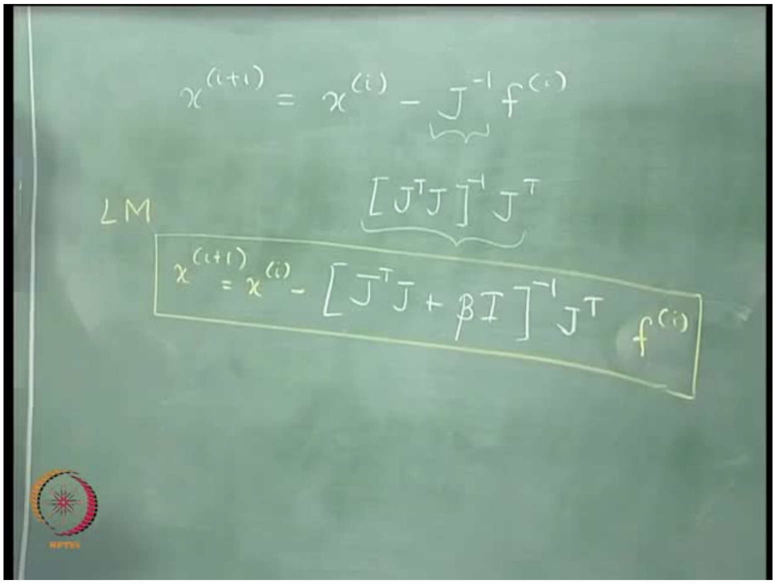

And one of the more straight forward ways of getting around. And this this is basically using this result what the result that I am go to show next is is something that comes out of out of that out of this particular result itself is for a multi variable case what we had said was what we had derived is x i plus 1 was equal to x I minus J inverse f computed at at the value i.

This is what we had we had derived and this derivation work extremely well when as long as J was non singular. That means as long as the rank of the matrix j was equal to n this particular case work really well however, if the rank of the matrix J is not going to be is not going to be equal to l. Then we need a slight modification to this keep in mind that this again again I am using pedagogical liberty is over here I am not using mathematically correct answer over here but, this we can actually write this as J transpose J inverse multiplied by J transpose.

As long as the rank of the matrix J is going to be positive as long as long as rank of matrix J is going to be equal to n this particular guy is going to reduce to nothing but, J inverse but, this is where a small trick comes in is instead of writing it in this particular form we write it as follows. We will write this as J transpose J plus beta times i inverse J transpose so, what we are done is we have introduce a small perturbation parameter beta over here.

That whenever this J transpose J starts getting close to being singular. We can use an appropriate beta value to give that small perturbation in the slope so, what happens when J transpose J is singular or when f dash is 0 is we reach a maxima of this sort and this is where basically the line the tangent line is parallel to the x axis. What this does is in the multi variable case it gives a slight slope and by giving it a slight slope we will prevent the overall method from stopping when J is not going to be invertible.

That is the whole idea over here and the expression remaining terms remain the same. As we had in the original version of Newton- Raphson's and that term that is going to be x i plus 1 is going to be equal to x i minus J transpose J transpose J plus beta i inverse of that multiplied by J transpose multiplied by multiplied by f of x i.

And this is basically called the luenberger mark what method of solving non-linear equations. We end our this particular lecture over here, what we have covered in this lecture is essentially multi variable extension for fixed point iteration, we saw that the fixed point iteration had a linear rate of convergence from multi variable system, we also saw the stringent conditions for the sufficient conditions for stability of the fixed point iteration. Then went over to multi variable case of Newton-Raphson's method and in the last ten or 15 minutes I give a very brief and a very superficial I may add introduction to the extensions that we can have to Newton- Raphson's method the Ralston's extension and the luenberger mark extension. The idea behind covering this extensions is for people who want to read further in order to get more more information about this you can you can now go ahead and read some of the literature and perhaps try to make sense of it.

Ok thank you very much.