Computational Continuum Mechanics

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Mathematical Preliminaries – 2
Lecture – 06-08
Linearization, Directional Derivative and Tensor Analysis

So, welcome to the next module of this course, which will be final module on mathematical preliminaries ok. So, there are three lectures planned in this module and as you can see these lectures will cover very important topics of Linearization, Directional Derivative and Tensor Analysis and also we will devote some time on working out some examples, so that you should be able to understand the theory much better.

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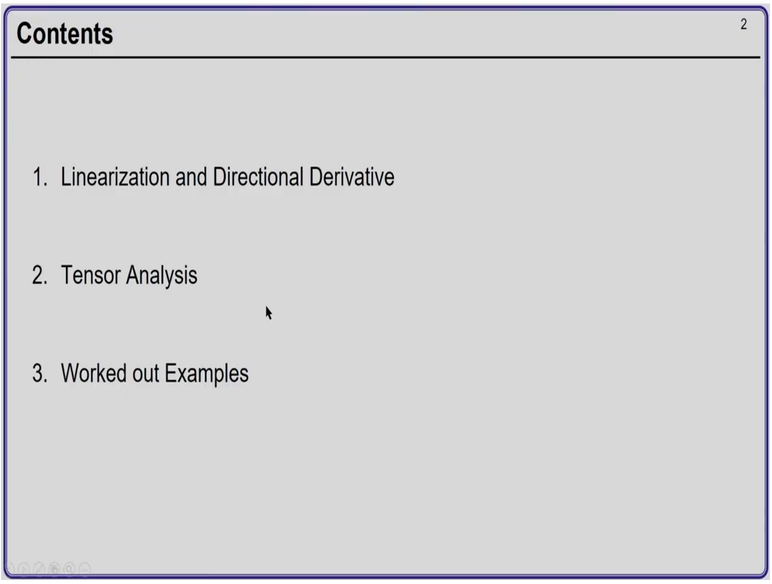

So, this is the content of this module. The first one is linearization and directional derivative. Followed by tensor analysis and then finally, we will look into the worked out examples to help you with the theory part.

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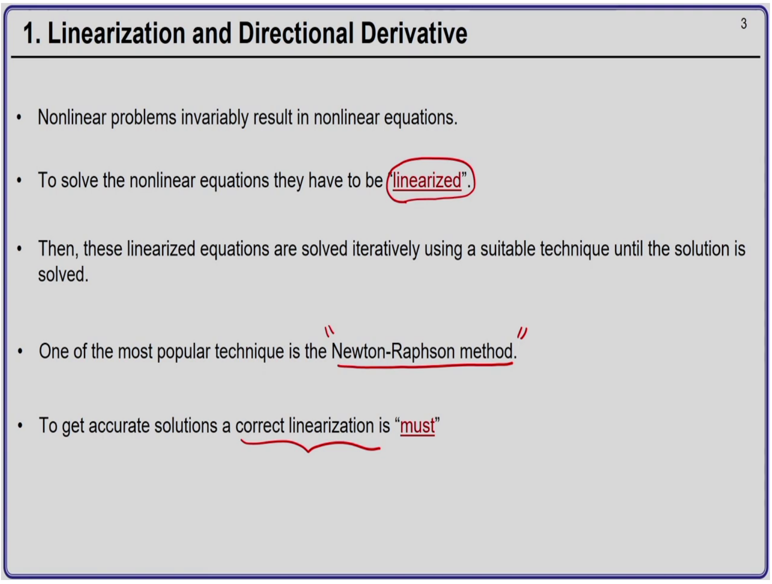

So, coming to the first topic, so, these non-linear problems will invariably result in non-linear equations ok. And these non-linear equations have to be solved by linearizing ok. That is what I have underlined here ok this term over here which is very important is linearization ok. So, you have to linearize these non-linear equations ok. And then once you have linearize these non-linear equations you have to solve these equations iteratively using a suitable technique and you have to do this until you have found out the solution ok.

So, one of the most popular technique is Newton Raphson method. Obviously, there are other techniques to solve non-linear equations, where you need not use any iteration. You can just keep on solving the equations. So, you linearize and then you can without employing Newton-Raphson method you can just solve that, but we will concentrate on method which use iterations to solve the system of non-linear equations and we will specifically focus only on Newton-Raphson method, ok.

So, to get the accurate solution for your system of non-linear equation you have to have a very correct linearization, ok. So, correct linearization is must for getting accurate solutions. What it means is if you do not linearize properly, it might happen that you might get a solution, but it will take much longer to get the solution; longer means in terms of the computational time or in the worst case you may not get any solution at all ok. So, it has. So, it is very essential that a correct linearization is carried out for Newton-Raphson method to work nicely, ok.

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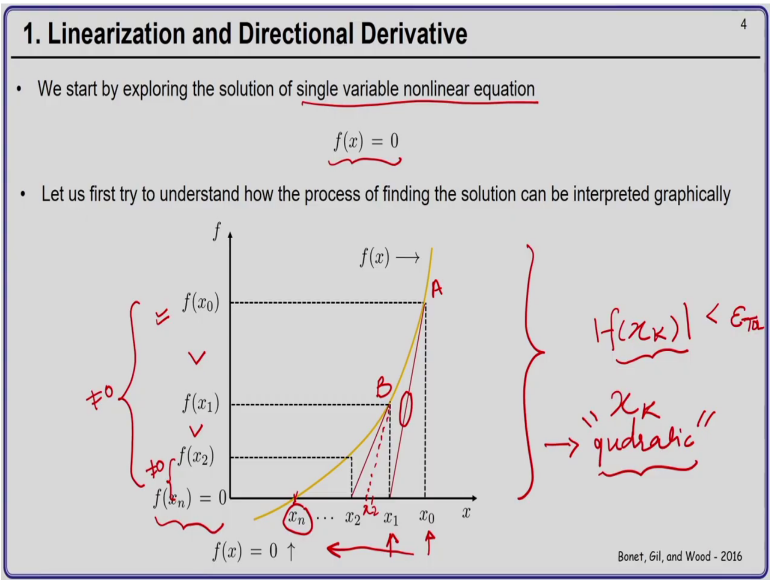

So, before we begin with system of non-linear equation, let us first start with exploring the solution of single variable non-linear equation, which is we have written here; f of x equal to 0, x is a variable ok. Now, our equation is f of x and now we want to solve this equation. What it means is we want to get the roots of this equation ok. So, we want to solve for those value f of x, for which f of x is equal to 0. So, before starting the mathematical details we first look into take graphical interpretation of how this solution for a non-linear equation is obtained using Newton-Raphson method.

So, as you can see here we have plotted for general function f of x which is shown here as this yellow line and the point at which this function cuts the x axis here that is where your solution lies ok. So, f of x equal to 0 is this point where the yellow curve intersects the x axis ok. So, now, to solve this equation the first thing that one should have is an initial guess ok. Initial guess means you do not have a idea about the solution, but you have some idea in which arrange the solution will lie, ok.

So, you have some idea of the solution. So, say x 0, say this is the initial guess that you start with and then as you know x 0, you know the value of f of x 0 ok. Now, you can see f of x 0 is not equal to 0 ok; so that means, x 0 is not the solution. So, what you do? What we do next is we make a tangent at this point. Let us call this point as A, ok. So, this red line is a tangent to the yellow curve at point A and then we know the slope of the line red line ok that is the derivative ok. Derivative of the curve at x 0 that is f dash x 0 and now we know this point also, the coordinates of this point.

So, we know the equation of red line and using that we can find out where this red line cuts the x axis. Let us say this point is x 1 ok. Now, again we can compute the value of the function at x 1 ok. Say this is the value of function f x f of x 1, ok. Now, we notice that although the value of the function is still not 0, but this value of the function f of x 1 is less than f of x 0, ok which means our new approximation of the solution x 1 has reduce the value of the function ok. So, we are approaching in the correct direction.

So, now, since we still not reached 0 then what we do? We follow the previous procedure. At say this point is B, now again at point B we make a tangent ok. And knowing the slope of the red line and the coordinates of point B, we can compute the intersection of the red line with the x axis. Let us say it cuts at value x equal to x 2.

Now, again I can check the value of the function f of x 2 ok. So, I can check the value of the function f of x 2 and you can see here that again f of x 2 is not equal to 0, but obviously, f of x 2 the magnitude or the value is less than f of x 1 ok. So, again we are reducing the value of the function ok. So, so on we keep on repeating this. So, we go to x 3 x 4 and we keep on doing this till we reach our point of interest which is this solution ok; f at say nth step we read the solution where f of x n is equal to 0 ok.

So, as soon as we reach f of x n equal to 0, we know that x n is our solution ok. So, that this graphical illustration shows how the Newton-Raphson procedure actually works ok. Now, the thing to notice when you are applying Newton-Raphson procedure over computer you may not actually get 0, ok. You may get a very small number maybe 10 raise power minus 9, 10 raise power minus 10 or something like that, but we will not actually get 0 ok.

So, we have certain criteria. We say that whenever say f of x k becomes less than say some value epsilon tol; tol is for tolerance ok. So, when the magnitude of the function at k-th point x k is less than our specified tolerance ok, so, this tolerance has to be given by the user who is using this procedure and when whenever this value becomes less than this tolerance we say that our solution is x k ok.

Now, the important point to note about this Newton-Raphson procedure is if you are nearer to the root, as you go nearer and nearer to the root that is as you approach the solution the rate at which the convergence is achieved is quadratic ok. So, if you are far away from the root say x 0 was far away from the solution that we were seeking then initially, the convergence will never be quadratic, but it might be linear what is called linear ok. But, as we approach towards the solution the last fewed steps of Newton-Raphson will actually show you that it converges what is called quadratically, ok.

So, that is one of the feature of Newton-Raphson procedure. And if you have computed your tangents that is slope of this red line if you computed this tangent accurately then this quadratic convergence is guaranteed. However, you will notice that even if say for example, at point B, you did not calculate the tangent accurately and say you calculated something like this then instead of reaching x 2 you would have reached a point x 2 dash, but still you have moved closer to the root or the solution x n, ok.

So, even if you have a wrong tangent it does not mean that you will not get a solution ok. You might still be able to get the solution, but your, the rate at which you will approach the solution will not be quadratic. You will take much more number of steps to achieve the solution that you have to remember. So, the fact that I mentioned in the previous slide, so, to correct to get the correct and accurate solution and ensure to ensure the quadratic convergence of Newton-Raphson procedure, it is necessary that you calculate the tangents of this Newton-Raphson procedure very accurately, so that I mean it means the linearization has been done very accurately ok.

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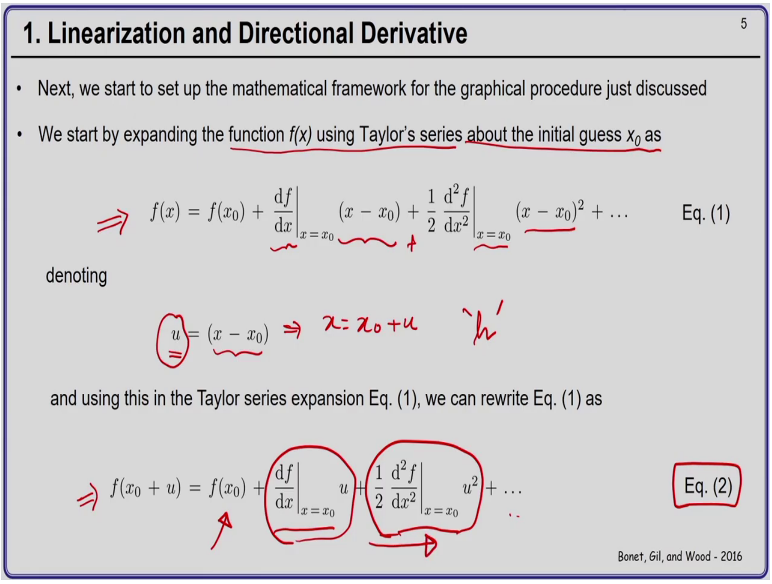

Next, we move to the mathematical framework for the graphical procedure that we have just discussed ok. So, now, what we do? We start by expanding this function f of x using Taylor series about our initial guess x 0, ok. So, equation 1 here shows that Taylor serious expansion of the function about point x 0 ok. So, f of x is equal to f of x 0 plus d of df by dx evaluated at x equal to x 0 into x minus x 0 plus 1 by 2 d square f by d x square evaluated at x equal to x 0 into x minus x 0 the whole square plus and so on.

You will have quadratic curve you have you will have quartic term like this ok. Now, if you denote x minus x 0 as u, which means x is x 0 plus u and if we use this in equation 1 then we can rewrite equation 1 as f of x 0 plus u equal to f of x 0 plus d f by dx evaluated at x equal to x 0 into u plus 1 by 2 d square f by d x square x equal to x 0, evaluated at x equal to x 0 into u square plus higher order terms ok. Now, the question you might raise at this point or your doubt might come why we have chosen this symbol u.

Because in undergraduate books on numerical analysis mostly this term h or the symbol h is use, but we have specifically chosen u because as we move later on in this course you will come to signify displacements ok. So, it is if we use this symbol here it is much easier to understand later because instead of this scalar u will have vector u which will be a bold. So, it is become very easy to understand much easier to understand ok.

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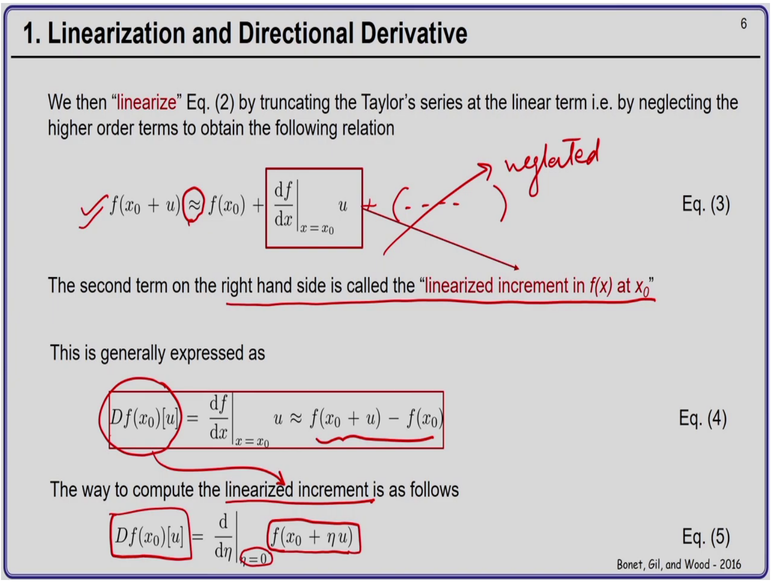

So, now you get this equation 2 over here. Now, what we do is we linearize equation 2 ok.

So, how do we linearize equation 2? You would have seen that the first term on the right hand side is a fix value ok. It is the value of the function at x 0. The second term, it is a linear function in u ok. It is a linear function in u because u has a power of 1; this df by dx evaluated at x equal to x 0 is a also known value, but u is unknown for you right now. Similarly, the third term is a quadratic term where u is u square, therefore, it is a non-linear term in u square.

So, all the terms beyond this linear term are non-linear terms ok, non-linear in u they are all non-linear in u. So, to linearize what we do is we neglect the higher order terms ok; terms containing u square u cube and henceforth that we neglect in equation 2. And then what we get is the left hand side will be approximately that is why you see instead of the equal sign now we have the approximation sign. So, f of x 0 plus u will be approximately equal to f of x 0 plus df by dx evaluated at x equal to x 0 into u and all the higher order terms which were here have been neglected.

We have all neglected the higher order term ok. So, this second term were on the right hand side is what is called the linearize in increment in f of x at x 0. So, this is the term in this bracket or this box red box is call the linearize increment in f x at x 0. So, this term on inside the red bracket is usually denoted by D capital D f of x 0 and then there is square bracket u equal to d f by d x x equal to x 0 into u, which from the third equation is nothing, but f of x 0 plus u minus f of x 0 ok.

So, this is a standard convention which is I have written here. This is standard convention and how do you compute this d of fx 0 at square bracket u? So, this square bracket does not mean that x 0 is multiplied by u it has a different meaning ok. So, whenever in this course we use square bracket, it does not mean you have to open up the bracket there is a special meaning for these kind of brackets, ok. So, the way you compute this linearize in increment which is this term over here is as follows ok.

So, what you do? You take a function and replace x by x 0 plus eta times u ok. So, if you have your function in x, what you do? You substitute x equal to x 0 plus eta times u and then what you do is take the derivative of that function with respect to eta and then finally, substitute eta equal to 0. Once you have done this you will get the linearize increment of f of x at x 0, ok.

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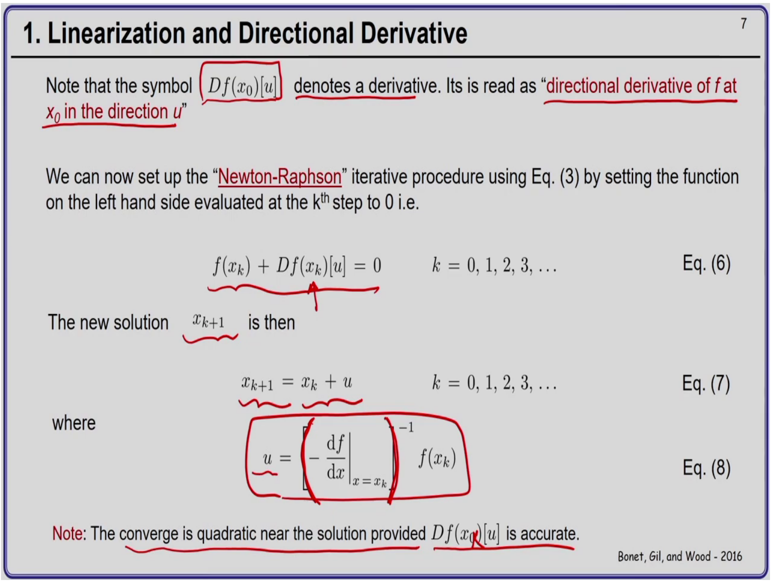

So, you have to note that this symbol D of f of x 0 at u denotes a derivative and the way it is read is directional derivative of f at x 0 in the direction u, ok.

So, whenever you see this term D of f x 0 at u ok, it is read as directional derivative of f at x 0 in the direction u. So, now, we can now set up the Newton-Raphson iterative procedure using equation 3 ok. So, what was equation 3? That was equation 3 ok. So, to set up Newton-Raphson procedure the left hand side of equation 3 is set to 0 and instead of x x equal to x 0 we put x equal to x k. So, we have f of x k plus the directional derivative of the function at x k evaluated in the direction u where k goes from 1; 0, 1, 2, 3, ok.

So, when k is 0 you have f of x 0 plus D f of x 0 at direction u. When k is 1, you have f of x 1 plus D f of x 1 in the direction u equal to 0 like so, on. And then what is x k plus 1? The new solution x k plus 1 will be simply x k plus u, where k goes from 1 to u ok. In this way you can set up the Newton-Raphson procedure. So, what we do? We start with k equal to 0; k equal to 0 you have x 0, ok. So, now, you compute u using this formula ok. So, this formula you can obtain from equation number 3.

So, u will be minus of d f by dx evaluated at x equal to x k raised to power minus 1 ok. So, there is a square bracket. So, let me just make it a other kind of bracket because I told square bracket will have a special meaning ok. So, you compute df by dx at x equal to x k ok, take the negative of it, take the inverse and then multiply it by f of x k. You will get the value of u ok. So, at k equal to 0 x 1 will be x of x 0 plus u then you recompute for x 2 x 3 and so hence so on and you stop when f of x k becomes less than a tolerance value ok.

So, the important point to notice the convergence will be quadratic near the solution provided the directional derivative of the function at x 0 or say x k is accurately computed ok. If you are computed your directional derivative accurately its guaranteed that you will converge quadratically near the solution ok.

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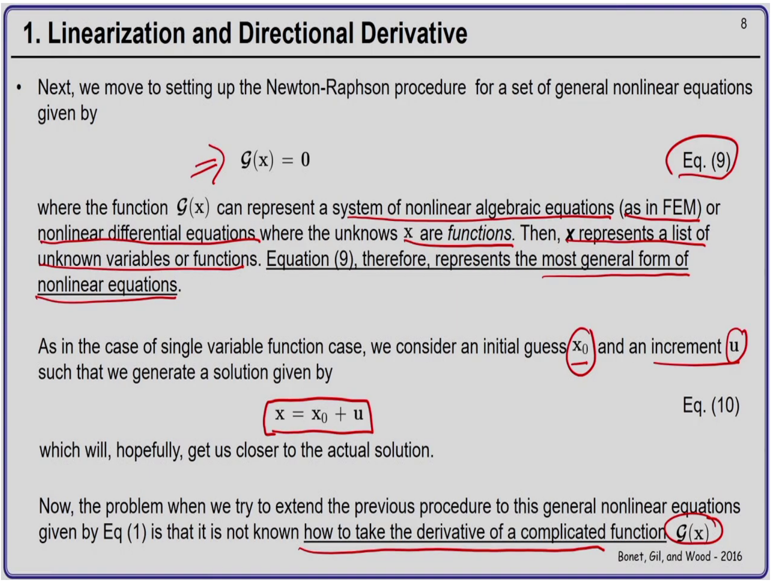

Next we move towards setting up the Newton-Raphson procedure for a set of general non-linear equations, which are given by this G of x equal to 0. Now you notice instead of scalars, now, we have bold symbols. Scalars were simple non bold symbols. Now, we have bold symbols and where this function G of x may represent a system of non-linear algebraic equation as one would get in finite element method or they may represents non-linear differential equation where the unknown x can be functions, ok. So, equation 9 is very general right now. It can represent system of non-linear algebraic equations or it may also represent non-linear differential equations, ok.

So, therefore, x represents a list of unknown variables or functions. Therefore, equation 9 represents the most general form of non-linear equations ok, that is the most general form and when we go into worked out examples you will be able to see it more clearly ok. Now, we want to solve this general non-linear equation ok. So, we again as was in the case for function or single variable we take an initial guess x 0 and we take an increment u ok. Now, we have x 0 which is bold which is some scalar and increment u which is also bold which means ok, it is a vector sorry x 0 is a vector.

So, now, we can generate a new solution x as x 0 plus u with the hope that when we do x 0 plus u ok, we will be getting closer to the solution ok. So, now, the problem right now is when we try to extend the previous procedure which we did for a single non-linear equation to this general non-linear equation given by equation 9 over here, it is not clearly known how will you take the derivative of a complicated function G of x ok.

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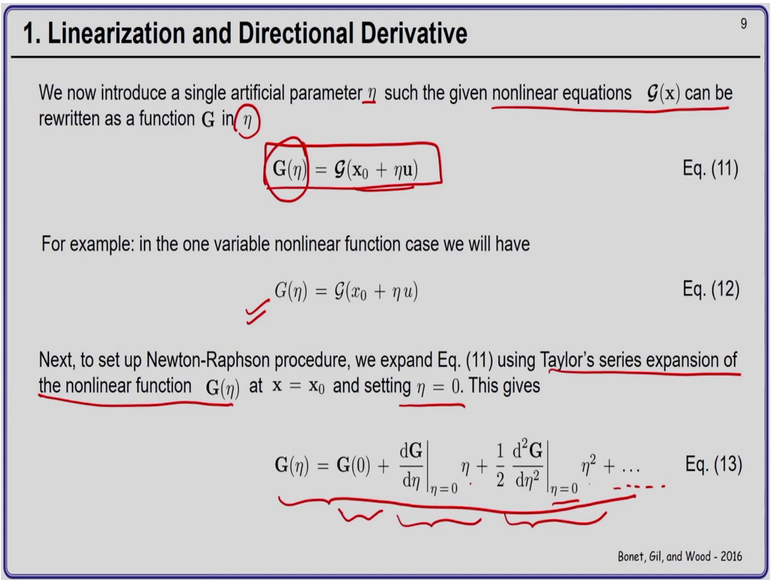

So, to do this what we do is we introduce a artificial parameter call eta ok. Remember our initial guess is x 0 and say we want to move in a direction u, arbitrary direction u that will take us closer to the solution. So, in a way we know x 0, u is what we want to find out. So, what we do is we rewrite our given non-linear equation G of x in terms of eta as given by equation 11 ok. So, we substitute instead of x we substitute x 0 plus eta u. So, what we get is a non-linear equation solely in terms of eta which is on the left hand side of equation 11, ok.

So, for one variable non-linear equation this would be like what is shown in equation 12 ok. Now, what we do is we take the Taylor series expansion of the non-linear function G of eta in equation 11 at x 0 and then setting eta equal to 0, ok. So, this is the Taylor series expansion of G of eta about x equal to x 0 and setting. So, we; so, G of eta is G of 0 plus d G by d eta evaluate eta equal to 0 into eta plus 1 by 2 d square G by d eta square evaluated at eta equal to 0 into eta square plus higher order term. Again you can see the second term is a linear term in eta that is third term is a non-linear term in eta. The first term obviously is known at eta equal to 0 ok. So, eta equal to 0 is basically x equal to x 0 ok.

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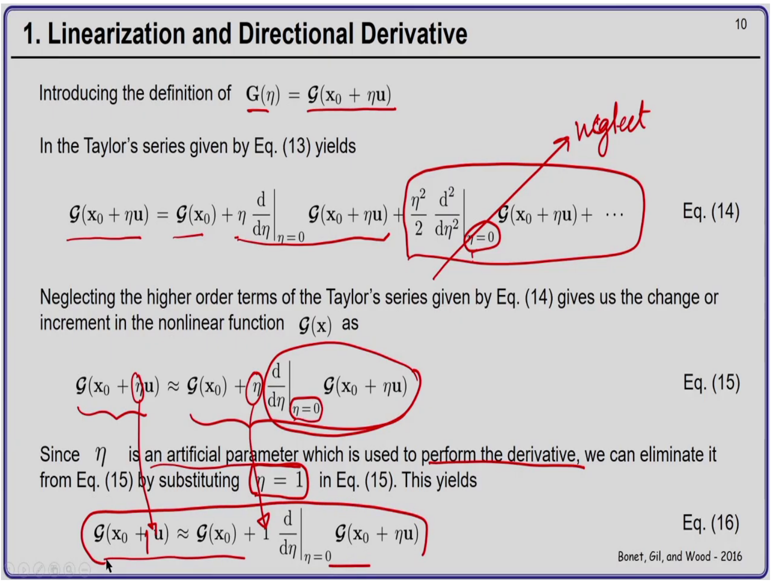

Now, we can introduce our definition G of eta was G of x 0 plus eta u ok. So, when we introduce this in equation number 13 which was there on the previous slide we can write G of x 0 plus eta u as G of x 0 plus eta d by d eta evaluated at eta equal to 0 of G x 0 plus eta u plus eta square by 2 d square by d eta square of G x 0 plus eta u evaluated at eta equal to 0 plus so, on ok. Now, we as we did in a single non-linear equation case we will neglect these higher order terms ok. What we will do is will neglect these higher order terms ok.

So, if you neglect the higher order terms, so, the left hand side will be approximately equal to G of x 0 plus the linear term in eta ok. Now, the problem here is we have unknown eta and we also have unknown u the direction in which we want to get the solution. It is the direction u is the direction which will take us closer to the solution because eta was an artificial parameter which was only used to perform the derivative. So, we can simply eliminate eta from our equation number 15 by just substituting eta equal to 1 ok.

So, when we substitute eta equal to 1, so, this eta will be equal to 1 and this eta will be equal to 1 ok. So, the eta here ok. So, this is no eta in this term because eta has been substituted with 0 ok. So, there is no eta here. So, what we get here is this equation 16, ok.

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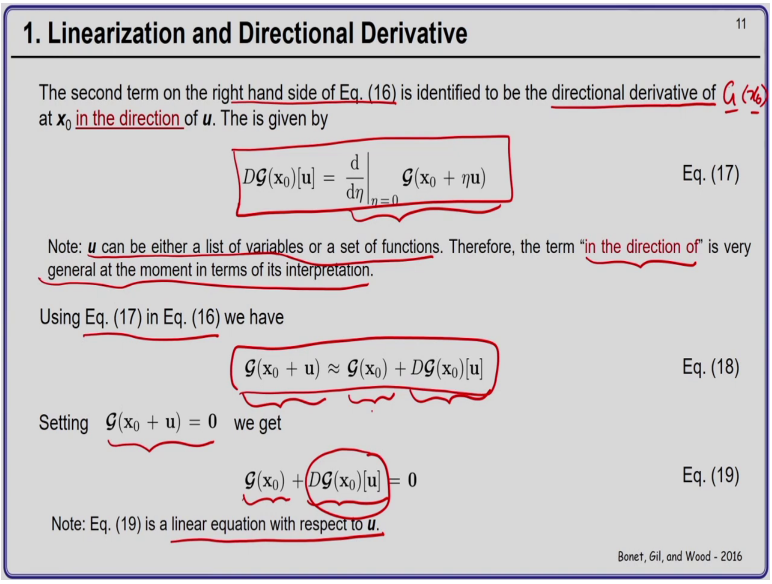

Now, this second term on the right hand side of equation 16 is what is identified to be the directional derivative of x 0 of G directional derivative of G of x 0 at x 0 in the direction of u and this is written as d G x 0 in u DG x 0 evaluated in the direction u and this can be is calculated using following expression on the right hand side ok.

So, you write the system of I mean you write the non-linear equations by substituting x as x 0 plus eta u then you take the derivative of that with respect to eta and then finally, you substitute eta equal to 0. So, this will lead to if this will give you the directional derivative of G at x 0 in the direction u, ok. So, you have to note that u can be either list of variable or a set of functions. So, therefore, when you are using this term in the direction of right now, is a very general term at the moment in terms of its interpretation ok.

So, I mean if you ask what is direction in the direction of a function, I mean it does not actually mean anything. That is why we when we say in the direction of therefore, its meaning is very general at the moment ok. Now, when you use equation number 17 in equation 16 on the right hand side in right hand side of equation 16, we substitute. We will get the new approximation of the function value G of x 0 plus u as the old value of non-linear equations at x 0 plus a linearized approximation DG evaluated at x 0 in the direction u, ok.

Now, if you set the left hand side equal to 0, then you get G of x 0 plus directional derivative of G at x 0 in the direction u equal to 0 ok. Now, this directional directive of G at x 0 in the direction u is a linear function is linear in u ok. So, this equation 19 is a linear equation with respect to u. So, you can basically solve for u and this will help you set up the Newton-Raphson procedure ok.

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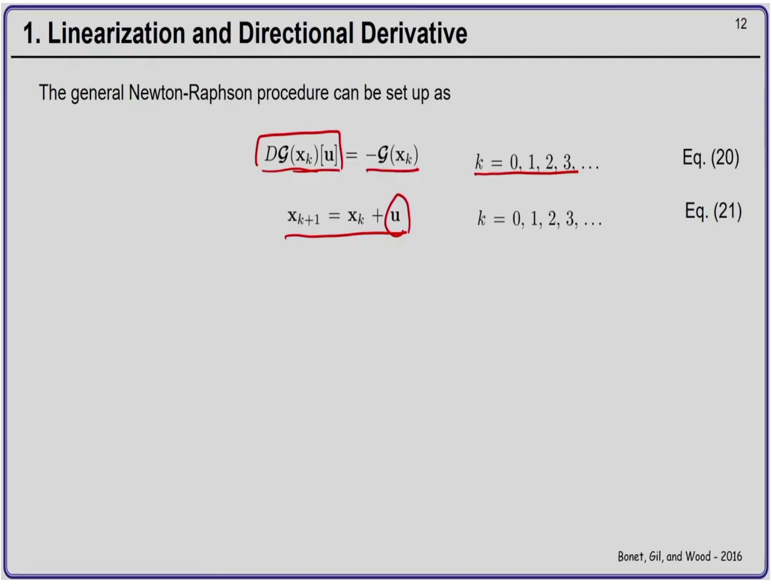

So, like previously we replace x 0 by x k a general kth step and we write you want to solve DG, directional derivative of G at x k in the direction u will be equal to minus of G evaluated at x k, where k goes from 1 2 0 1 2 3 and then the new solution x k plus 1 will be the old solution x k plus the direction u which has been computed in from equation number 20 and then you iterate ok. So, you start with x equal to 0 you start with a k equal to 0 sorry and then you have x 0 you compute u get the value of x 1 you go back check the convergence criteria.

And if the criteria is not fulfilled then you compute x 1 x 2 then you again compute u and then compute x 2 as x 1 plus u and you keep on doing this till you achieve your convergence criteria ok. So, this establishes the Newton-Raphson procedure for non-linear equations given by G of x equal to 0 ok.

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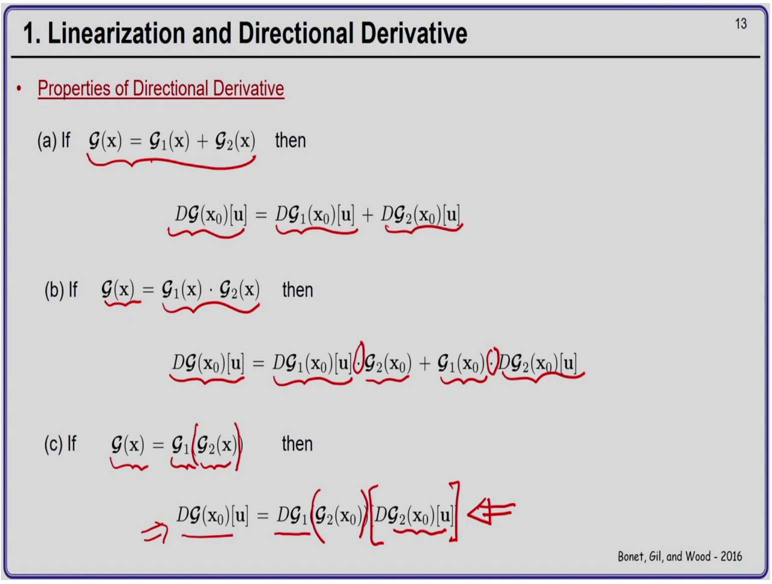

So, there are some properties of directional derivative which will be needed in the worked out examples that we will do and we will revised these three properties. The first one is if the given non-linear equations can be written as addition ok or the sum of two set of non-linear equations G 1 x plus G 2 x then the directional derivative of G at x 0 in the direction u will be the directional derivative of G 1 at x 0 in the direction u plus the directional derivative of G 2 at x 0 in the direction u ok.

The next is if you can write your given non-linear equation as a product of two functions G 1 and G 2, so, G 1 x into G 2 of x, then the directional derivative of G at x 0 in the direction u will be the directional derivative of G 1 in the direction u evaluated at x 0 times G 2 evaluated at x 0 plus G 1 at x 0 times directional derivative of G 2 at x 0 evaluated in the direction u.

Now, this dot I mean this dot that you see here ok, again its very general has a very general meaning right now. I mean it does not actually mean the multiplication ok. The last property is suppose your G of x is G 1 function of G 2 which is again function of x, then the directional derivative of G at x 0 in the direction u will be nothing but the directional derivative of G 1 at G 2 evaluated at x 0 in the direction in the direction of the directional derivative of G 2 evaluated at x 0 in the direction u, ok. So, understand it is a little bit confusing right now. So, next we will see this last property in much more detail in the next slide.