**Numerical Methods and Simulation**
**Techniques For Scientists And Engineers**

**Saurabh Basu**
**Department of Physics**
**Indian Institute of Technology- Guwahati**

**Lecture 04**
**Newton Raphson Method (Examples)**

So, let us carry on with the solution of these equations numerical solution of these equations. We have seen two methods ah namely the bisection method and the secant method. We saw that the bisection method suffers from the fact that ah first it has slower convergence it is a linear convergence and the other one is that you have to give two values which subtend the root. If you miss the root and give two values which they do not subtended root.

And in that case bisection method will not work and in fact you have to give again new choices. The secant method is slightly better which requires you to which has a faster convergence faster than linear convergence. Now let us look at the Newton Raphson method.

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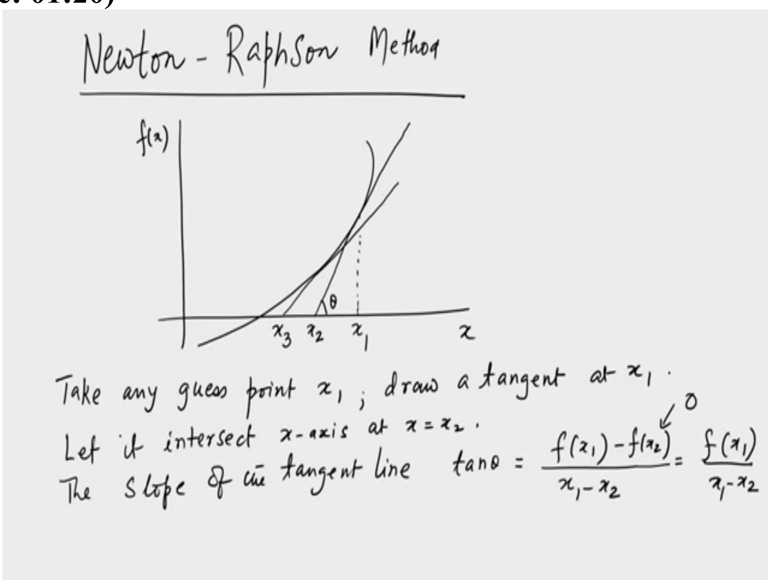


So, what is this method how do we use it in order to calculate the root of a given equation okay, ah it of course requires only one value to guess so it starts with just one value. And so let us just consider the following graph for fx, so this is your ah fx okay so this is fx as a function of x and let us take a value let us call this value as x 1, that is the guessed value. And what it requires is that you need to calculate or rather draw the tangent at this point.

And not a very good tangent but that is just a freeway every Android it just touches at this particular point at x 1. And then let us call this angle as theta and then of course we get so wherever the tangent cuts the x-axis let us call that points as x 2 and take this point f of x 2 which is which is here and then draw another tangent and so on okay. So, if you see that we are coming closer to the root.

And so it requires the value of the function at a given guess point and then requires you to calculate the slope at that particular point okay. So, this is how we come closer you see x 1 was the guessed value and then it became x 2 and then it became x 3 and so on. And of course it also has limitations which we are going to come to, but this will be shown to have a faster as compared to the bisection or the secant method.

So, take any point writing it for your convenience any point let us call it a guest point x1 that is a value of x then ah draw a tangent ah at x1 then ah of course ah let it intersect x-axisah at x equal to x 2, now the slope of the tangent line which is nothing but tan theta this is equal to f of x 1 x 1 – x 2 of course it is f of x 2 as well but then you know f of x 2 is equal to 0, so this is equal to 0 so we can simply write it as f of x 1 and x 1 - x2 ok, f of x 2 is 0.

Because you see that the function is cutting the line at x 2 at exactly you know x equal to x 2. So, this is the so that is the value of this or rather that that is the slope of the tangent line.

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Solving for $x_2$,

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} \Rightarrow \text{Newton Raphson (NR) formula}$$

Iterating it $x_3 = x_2 - \frac{f(x_2)}{f'(x_2)}$

$\vdots$

$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}} \rightarrow \text{NR formula.}$$

If $f'(x_n) = 0 \Rightarrow$ One has to go lack and look for a new guess and iterate the process again.

Now if you solve for solving for x2 one gets x 2 equal to x 1 - f of x 1 divided by f prime of x 1 and this is precisely called as the Newton Rapson and in short we will call it as an NR formula ok. So, this is the iteration formula. So, what it means is that so if you iterate it ah x 3 becomes equal to x 2 - f of x 2 divided by f prime of x 2 and hence basically you get a new root after every iteration which is equal to the old root minus the value of the function at that old point or root point divided by the slope at that particular point.

So, this is; so if you iterate it your x i + 1 or x n + 1 if you like it is equal to x n - f of x n divided by f prime of x n, so let us box this and we will use this like NR formula it is the same as the above excepting that it is written for ah after n iterations ok. So, this is the value of the new root of course there could be a problem the problem occurs when f prime of x n goes to 0 okay. So, if that happens that is this goes to 0 then of course you see that denominator becomes 0 means it blows up so you would not get any; so you will get an infinity for the new root which is of course ah not an allowed solution for a given problem.

So, in that case one has to go back and look for a new guess and iterate the process again. So, let me quickly take you through this thing that you have a curve and you want to know the solution of that equation it could be highly nonlinear, you need to make a guess and of course you need to make also a tolerance because once the actual root is reached or if you are doing it several times ah the iteration you have to understand that when to stop that iteration.

And that you have reached the final answer for your particular question that you are attending to. And in order to do that you your x n + 1 – x n should give you a tolerance number if the x n - 1 – x n the modulus value of that or the absolute value of that falls below the tolerance then you say that I am done with my numeric computation of the root and that is the value of the root either way x n or x n + 1.

So that you need to give a tolerance which is come going to come to that, so let us look at a simple example.

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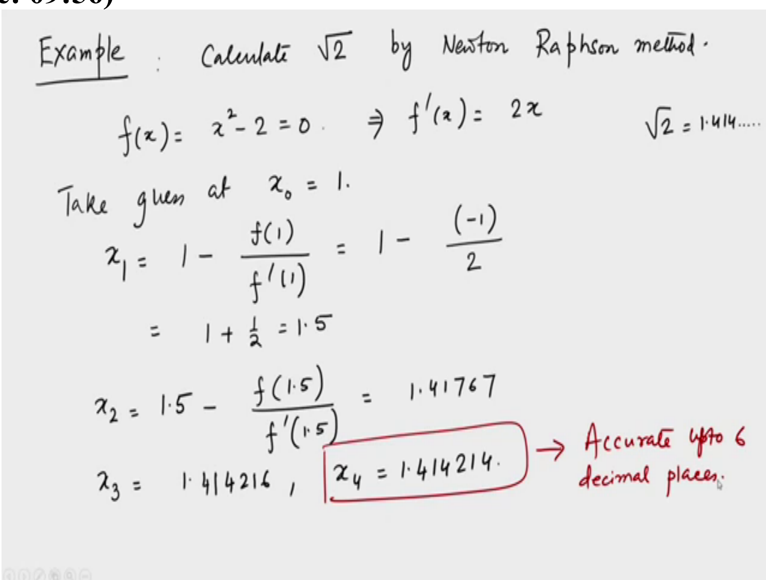


Says calculate root over 2 by Newton-Raphson method, so that of course tells you that you have fx equal to x square - 2 equal to 0, so that you have to solve this equation in order to find the value of square root of 2. Now ah of course this gives that the f prime x is equal to 2 x ok, so if

I take guess as 1 that is your the first value that which we are taken say call it x 1 or you can call it x 0 that is a 0th value it is equal to 1.

Then what we can do is that we can calculate x 1 which is equal to 1 - f of x 0 which is 1 and f prime of x 0 which is this which is f prime of 1, so it is 1 - f of 1 is equal to - 1 and f prime of 1 is equal to 2 because if you put x equal to 1 there. So, this becomes equal to 1 + 1/2 which is equal to 1.5, so that is the second in the second iteration you get a value which is 1.5. If you want to iterate it further if you feel that that value has not reached you know the value this is like 1.414 etcetera and then so basically this is very well known 414 with I leave those extra digits here.

So, now your x 2 will simply be equal to x 1 - f of x1 which is 1.5, so let us write 1.5 in that case and this is 1.5 divided by f prime at 1.5 and this ah comes out to be 1.41767 similarly if you iterate your x 3 becomes equal to 1.41 please take these numbers as you practice this and then again doing it 1 it is 414214 and it is pretty much accurate till 6 decimal places. So, we can take this x 4 to be the root for so that gives you only 3, 4 iterations of course the problem is very, very simple.

So it gives you a root in only in something like 3, 4 iterations it gives you a value which is fairly reliable ah and ah very close to the exact value.

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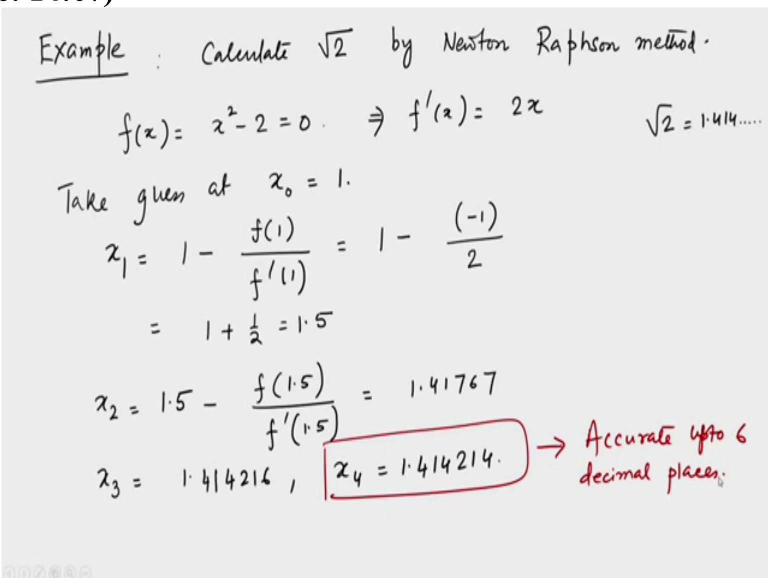


So, let us look at the algorithm of this Newton-Raphson method. So, the first thing is that assign an initial value of x that is x 0 and tolerance let us call it tol, so this tolerance will decide ah when to terminate the numeric computation of the root okay. So, this is that reason; for the tolerance, so these are steps, so let us call them as steps. So, step 1 and then step 2 is that of course evaluate f of x 0 and f prime of x 0 that is at the initial value.

And then obtain an improved estimate of x 0 by using NR formula and so this will become equal to x 1 equal to x 0 f of x 0 divided by f prime of x 0, so along with that of course you should check accuracy that is the 2 successive values whether they are other ah relative values are coming closer or lesser than the tolerance which means that check for x 1 – x 0 divided by x 1 the absolute value of that whether it is falling below the tolerance okay tol.

And if it is yes you stop okay and if no go back to step 3 and then of course stop once you find that this condition is made. So, this is the simple algorithm of this method is fairly easy method however and it has a lots of merits. So, let us look at an example another example of this Newton-Raphson method. These are simple examples but these simple examples are nevertheless very indicative of the efficiency of the method.

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Example

$$e^{-x} - 5x = 0.$$

$$f(x) = e^{-x} - 5x. \Rightarrow f'(x) = -e^{-x} - 5$$

$$x_{i+1} = x_i - \frac{e^{-x} - 5x}{-e^{-x} - 5}$$

$$x_{i+1} = x_i + \frac{e^{-x} - 5x}{e^{-x} + 5}.$$

So let us look at this equation which is it is exponential - x - 5x equal to 0 so what we have been given is that this is equal to - 5x ok and that of course gives me that f prime x which is the slope or the derivative which is equal to - exponential - x and - 5 okay. So, what is my x i + 1 that is equal to x i - exponential - x - 5x divided by - exponential - x - 5 and this tells you that it is equal to + exponential - x - 5x divided by exponential - x + 5 and so on.

So, this would be the formula for iterating the roots and then you take a value of guessed value initial guess value for x and one would get successive values. And then you also decide on a tolerance and find that I mean a check for the relative difference between the two roots or ah in two successive iterations and if you find that that value is falling below the tolerance are falling lower than the tolerance then the computation is complete okay.

So, let us give another example which are you know ah ah sort of is a quantum mechanics one often encounters this and sometimes ah even students have difficulty with the quantum mechanics question itself not with regard to solving it numerically but with regard to understanding that what bound states etcetera mean.

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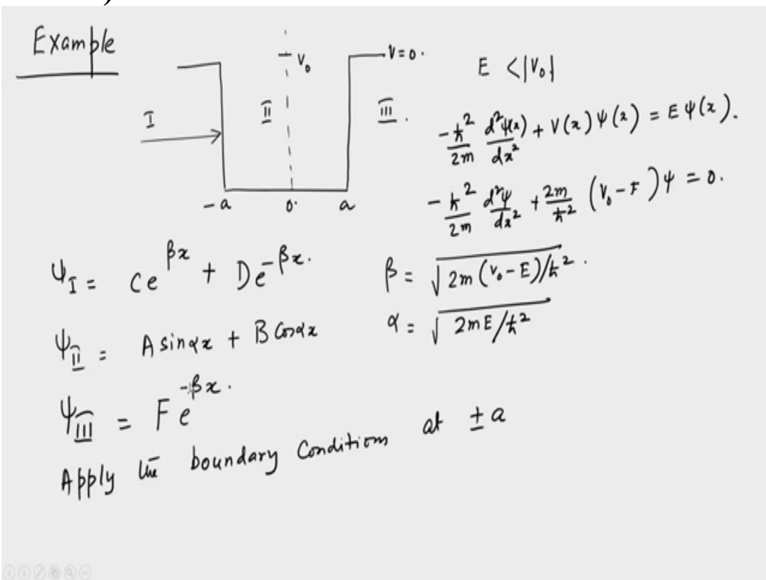


So, let us give an example. So, let us take a potential well it is not a potential barrier it is a finite potential well of some certain width let us call it from - a to + a with the 0 lying in between and ah this has a value equal to call it a v 0 there is a region one this is the inside of the well it is called region 2 and it is region 3 is here. Suppose you have an energy which is lower than so your E is actually lower than v 0 and of course your v 0 is a negative here.

So, this is v equal to 0 rather and we can we can solve this problem it is a so we can solve the Schrodinger equation just to remind you is written as this and it is a d 2 psi dx 2 + v of x psi of x, so let us call it a psi of x it is a one dimensional problem. And this is equal to E psi of x ok. So, it is quite simple to solve ah the potential is 0 outside and it is equal to – v 0 inside and C in region 1 and 3 one can put the potential equal to 0 and in the region to the depth is v 0.

So, we can call these and the energy of the particle is actually lower than the magnitude of this or let us call it this and so on, I will not go through the details of the solution I will simply write down the solutions themselves. So, this particular will become equal to so 2 m d 2 dx 2 + 2 m by h cross square v 0 - E and psi and that is equal to 0, so we have a solution as psi 1 equal to C exponential beta x and D exponential - beta x beta being this constant for a given energy psi II where alpha is another constant which is given by; you should be able to find it in any quantum mechanics book.

Say for example Griffiths or even I mean any book any quantum mechanics book will give it. Psi III has a solution which is similar to 1 accepting the fact that it does not have a reflected component such as 1. So, it is in 3 it is like okay and one can apply the boundary conditions at + and - a maybe there is a - sign here.

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At $x = -a$

$$-A\sin\alpha a + B\cos\alpha a = Ce^{-\beta a}.$$
$$\alpha A\cos\alpha a + \alpha B\sin\alpha a = \beta Ce^{-\beta a}.$$

At $x = a$

$$A\sin\alpha a + B\cos\alpha a = Fe^{-\beta a}.$$
$$\alpha A\cos\alpha a - \alpha B\sin\alpha a = -\beta Fe^{-\beta a}$$

The wave functions have different parity.

Even States $A=0, \; B\neq 0, \; C=F \Rightarrow \alpha\tan\alpha a = \beta.$

Odd states $A\neq 0, \; B=0 \quad C=-F \Rightarrow \alpha\cot\alpha a = -\beta.$

And what one gets is the following, I am simply writing down the equations that are needed for us and how to arrive at those equations. So, at x equal to – a, so these are psi being continuous and psi dx being continuous and these are at x equal to + a okay. So, this problem of course has a finite parity. Parity means the inversion symmetry which means that because of the symmetry of the potential if you see the potential is symmetric about 0.

So, if this is called as an inversion symmetry or a parity and if the potential has that symmetry the wave functions actually pick up or rather pick up that symmetry and they split into two classes of solutions. One are called as one is called as the even parity states and the other is called as the odd parity States. And so the wave functions have different parity. So, the even states correspond to A equal to 0, B 0 equal to 0, C equal to F that implies C equal to F and it implies alpha tan alpha a equal to beta.

And the ah odd States we are coming to the interesting part of the question which we have to solve this corresponds to A not equal to 0, B equal to 0, C equal to - F and this is equal to alpha cot alpha a equal to - beta and you see this in your quantum mechanics book just let us just go to that why for even states you will have a equal to 0, because your solution is with the a goes with a sign. Now if x changes sin, sin changes sin as well right.

Because sin is an odd function cos is an even function. So, for even states we want the odd term to go to 0 so that is why A equal to 0, but B being associated with the cosine term and cosine being even that is if you change x to – x, cosine does not change sign which means cos of -theta equal to cos theta in that condition of course applying the boundary conditions your C becomes equal to F.

And what we get by from these two conditions is that the alpha tan alpha a equal to beta and similarly for the odd States when you want the even terms to go to 0, C acquires a value equal to –F. And similarly the bound states are given by these conditions.

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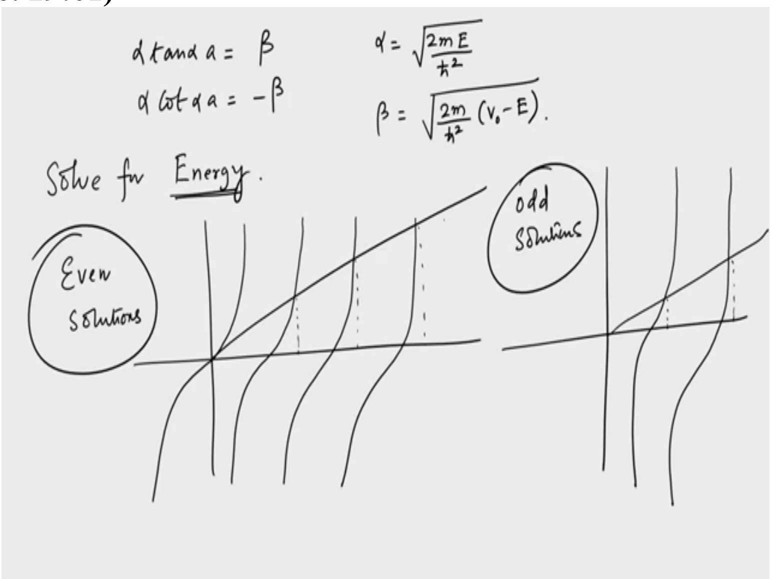


So, we have two equations which we want to you know so we have an alpha tan alpha A equal to beta and we have an alpha cot alpha A equal to – beta, remember your alpha equal to root over 2m e by h cross square and beta equal to root over 2m by h cross square V 0 – E, so you have to solve for; that is the whole idea of a quantum mechanical problem that we have to solve for the energy. And if you have to solve for the energy you see energy is there in both alpha and beta.

And it is not only there in alpha and B; and since alpha and beta occur at both sides of the equation. So, there are you cannot simply separate out the unknown on one side and writing all the known quantities on the other side both the sides of the equation on either side of the equality sign it involves these energy E. So, solving is somewhat non-trivial and also given the fact that this alpha is present in the arguments of both tan and cot.

And cotangent and that makes the problem even more difficult. So, the books you see the books in which they you know do it these are called as transcendental equation and the only solution that is possible or rather the only two methods that are possible a one being the graphical solution. So, let me plot for a given value of energy let me plot both the sides separately and see where they intersect okay.

And so basically this is what you will see that there are you know tan etcetera and so on. And this beta will of course if you plot it I mean suppose you plot that thing and say it goes like this so this is the say RHS okay. So, you get a solution here at the origin then you get a solution here and then you get a solution here and then you get a solution here. So, your energy of the particle will decide how many bound states are there okay.

So you may not have you know large number of bound States where as for the other solution these for the even solutions. And for the odd solutions because they involve cotangent, cotangent does not pass through the origin. So, you have so basically you will have again these as these values. So one very trivial information that comes out from this is that if you have infinitesimal energy that is if E is very small and negative you still have an even bound state.

If you go to that if your E is infinitesimally below 0 you still have the possibility of at least one ah bound state which is even bound state which if you does the wave function has a property that if you change x to - x it does not change sign that is called evenness. And but if you look at this plot you will not have a solution for an infinite as you will not have an odd bound state that is it will change sign on changing the sign of x.

It will not have such a bound state for infinitesimal small infinitesimally small energy. And which are fine of course we are we have learned that and is called a graphical solution but what about solving these equations using the numerical method that we have been exposed to for or reusing Newton Raphson's method.

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For a Computer it is more convenient to represent the equations as,

$\beta \cos\alpha a = \alpha \sin\alpha a$ for even bound states.

$\alpha \cos\alpha a = -\beta \sin\alpha a$ for odd bound states.

Even bound states,

$$\boxed{f(E) = \beta \cos\alpha a - \alpha \sin\alpha a.}$$

$$E_1 = E_0 - \frac{f(E_0)}{f'(E_0)} \qquad \left|\frac{E_{i+1} - E_i}{E_{i+1}}\right| < tol.$$

Of course for a computer it is more convenient to represent it as I mean the equation as the reason being that there are divisions by sine and cos, so we can simply write it as beta cosine alpha a equal to alpha sin alpha a for the even bound states. I hope this word even bound State is not bothering you once again I want to repeat it is a solution of this Schrodinger equation for the particle which has a property that if you change x to - x the wave function does not change sign that is called an even bound state or even wave function.

So, that bound state corresponds to a wave function and that is the function that we are talking about, it is a simple function I mean wave function is a quantum mechanical concept for us it is a simple function. So, these are simple functions and beta and alpha actually contains a within a square root. And for the other odd bound state which of course you know that it has a meaning that this is if you change x to - x then it will change sign for odd bound states.

So we could have started this problem here that take these two equations and find out the roots of these equations. But we wanted to give put it in perspective I mean this is basically very important for the physics students to know that this calculation of bound states. Because the scattering states are easier when you have a potential infinite potential well and things like that things are easier where you have solutions which are of sine and cosine.

But when you have these other kind of solutions then you have for these bound states and so to cast it in the form that we need to, so let us only do it for the even bound states f of E beta cosine alpha a - alpha sine alpha a and I would get a value of E the first iterative value of E from a guess value E 0 by calculating f of this divided by f prime of this ok. So, you can iterate it according to the Newton Rapson this equation and the you iterate it a number of times.

And also of course defines a tolerance so that you know when the root is reached so basically we will have E i + 1 – E i divided by a E i + 1 that is the relative value should fall below predefined tolerance and that tolerance of course depends on how accurately you want to get your root or depends on the particular problem that you are attending.

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## Convergence of the Newton Raphson Method

Let at the nth step $x_n$ is the estimate for root of $f(x)$

If $x_n$ and $x_{n+1}$ are close to each other, then use Taylor series.

$$f(x_{n+1}) = f(x_n) + f'(x_n)(x_{n+1} - x_n) + \frac{1}{2} f''(R)(x_{n+1} - x_n)^2 + \cdots \quad (1)$$

R is any point between $x_{n+1}$ and $x_n$.

Let us assume that the exact root is $x_r$. Also assume that $x_{n+1}$ is very close $x_r$, so that we can claim $f(x_{n+1}) \simeq f(x_r) = 0$

Putting $f(x_{n+1}) = 0$ in Eq. (1)

$$0 = f(x_n) + f'(x_n)(x_{n+1} - x_n) + \frac{1}{2} f''(R)(x_{n+1} - x_n)^2 \quad (2)$$

Let us look at the convergence of the Newton-Raphson method. We are testing this every time a convergence what is the error, how the error is reducing as you go from one iterative step to another iterative step and so on. And this is extremely important in the context of numerical methods where we need to make sure that the; we are doing the iterations and the errors are not increasing there in fact going down.

And how the errors are decreasing as you go from one iterative step to another will decide what is the most efficient algorithm for a particular problem to use. And so these are demonstrating the fact that a which method out of the 3 that we have talked about namely the bisection method the secant method and Newton-Raphson method which one is more accurate. So, in order to do this let us look at the let at the nth step x n is the estimate for root of a function f of x and of an equation f of x equal to 0 okay.

Now if x n and x n + 1 are close to each other, so we are assuming that the two computed values for the root in two successive iterations after a number of iterations they do not differ too much then use Taylor series which I believe you have read in your course of mathematics or even in some parts of statistical mechanics and physics or in different branches of engineering which is done to expand a function about a value which is a neighbouring value.

So f of x n + 1 is expanded about f of x n I will tell you what is R and then there are other terms but since x n is sufficiently close to x n + 1, I am stopping it at the quadratic level of this series R is any point between x n + 1 and x n, because they are close we can take the value at any point in between these two values and compute the double derivative at that point. So, there is a x n that I havee missed all right the thing is calculated or rather the slope is calculated at x equal to x n.

Now let us assume that the exact root is x r, r for the real root or something, also assume that x n + 1 is very close to the real root x r so that we can claim f of x n + 1 which is equal to f of x are equal to 0 because if it is a root then of course the value of the function will vanish there. Now importantly x n + 1 and x r are two different points which are neighbouring way nearby points.

But the values of the function add those two while those two particular points that is x n + 1 and x r the values are same but the points are not same that is what this is saying. So, if your f x n + 1 is equal to 0, let us call that as equation 1 putting f of x n + 1 equal to 0 in equation 1 we get 0 equal to f of x n + f of x n x n + 1 – x n + 1/2 of f R x n + 1 – x n square and we are neglecting terms from their own alright. Now so let us call this as equation 2.

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From the NR formula, $\qquad x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$

$$f(x_n) = f'(x_n)\,(x_n - x_{n+1}) \qquad (3).$$

Put (3) in (2),

$$0 = f'(x_n)(x_n - x_{n+1}) + f'(x_n)(x_r - x_n) + \frac{f''(R)}{2}(x_r - x_n)^2$$

$$0 = f'(x_n)\big(\underbrace{x_r - x_{n+1}}_{\varepsilon_{n+1}}\big) + \frac{f''(R)}{2}\big(\underbrace{x_r - x_n}_{\varepsilon_n}\big)^2.$$

$\varepsilon_{n+1} = x_r - x_{n+1}$

$\varepsilon_n = x_r - x_n$

$$0 = f'(x_n)\,\varepsilon_{n+1} + \frac{f''(R)}{2}\,\varepsilon_n^2$$

$$\varepsilon_{n+1} = -\left(\frac{f''(R)}{2\,f'(x_n)}\right)\varepsilon_n^2$$

Quadratically Convergent.

From the Newton Rapson formula, let us write it as NR as a brief, so f of x n equal to f of x n f prime of x n into x n – x n + 1 it is the same formula that we have written earlier x n + 1 this is that x n + 1 equal to x n - f of x n divided by f prime of x n, so this I have rearranged this to write it in this fashion. So, let us call that as equation 3, so put 3 into and we have a 0 equal to f prime of x n x n – x n + 1 or we have I mean this is equal to your n + 1 from this and a + f prime x n that is coming from the secant term here, this one.

So this is equal to x r - x and remember we have taken x n + 1 equal to x r and then we have the harmonic term which is 2 which is actually 2 factorial and – x n whole square. So, if you simplify this, this becomes equal to f of x n x r - x n + 1 as I said these two points are not same but the value values of the function and these two points can be taken to be same these are two neighbouring points and we also have the f R the double derivative of f evaluated at R and this is x r - x n whole square.

So, of course we have not substituted this to be equal to 0 but we have taken this if you look at it we have taken this x n + 1 equal to x r in the secant equation but or in the second term but have not taken in the first term we have still considered x r and x n + 1 to be different but this is what we actually call as the epsilon n + 1 that is the error at the n + 1 at step and this we call as the error at the nth step.

And it is very intentional to keep these things because these are errors these are extremely small quantities at the n + 1 at level and in order to find a relationship between the error at the nth level and the n + 1 level have taken these things that is we have you know these x n + 1 so here the x n cancels and one has a x r – x n + one which have not taken to be the same however in the other where there was xn + 1 and xn then we have taken x n + 1 as x r which is equal to x, x my or rather it has to be the other way around.

So, let us just epsilon n + 1 equal to x r – x n + 1 epsilon n equal to x r - x n, so this tells that 0 equal to f of x n epsilon n + 1 and + f this and epsilon n square there is a factor of 2, so epsilon n + 1 is minus the double derivative of the function evaluated at that r point which is between x n and x n + 1 it does not matter you can calculate it at any of these anyway these are number this this particular you know this is just a number so epsilon n + 1 goes as epsilon n square so it is a quadratically convergent let us look at what it actually means something to be quadratically.

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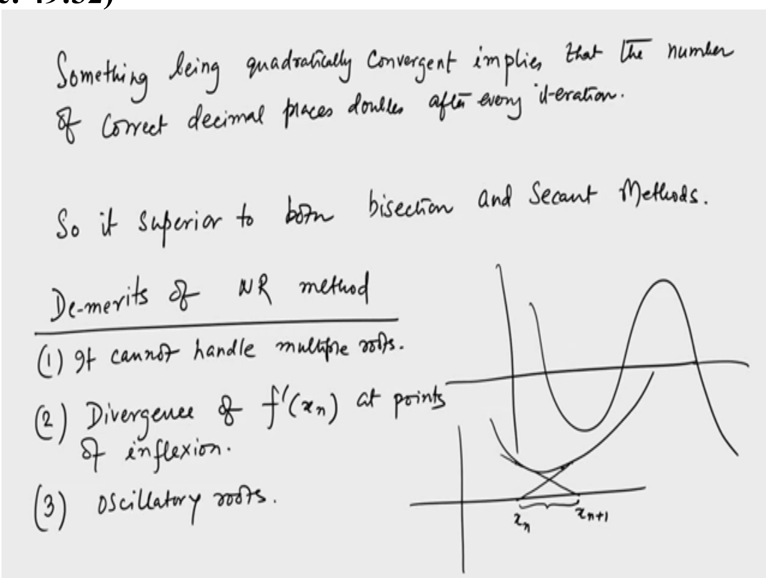


So, something being quadratically convergent implies that the number of correct decimal places doubles, doubles after every iteration okay. So, if at a particular iteration the number of correct decimal places correct means compared to the real root is 2 in the next it will be 4 and so on ok so that is what it means. So, of course superior to both bisection and secant method. Bisection has a linear and ii has more than linear but of course that is not here I mean not power of two less than a power of two is between one and two okay.

So what are the demerits of in our method of course which is very simple to understand it cannot handle multiple roots? What it means is that if you have a function which goes like this and so on so you have three roots so you have to have you can only handle one root at a time. The other is mainly related to ah the divergence of f prime x n the point of you know inflection. The third could be oscillatory roots that is if you have a situation which has a value like this then of a guess value here would give a slope here.

And then you have to consider at this point where it touches and then you will get a slope which is here so here the roots actually oscillate. So, this is say x n and this is x n + 1 they are completely in the different directions and of course this is this oscillatory solutions will cause confusion and will not let it converge. And of course the convergence is only quadratic and not powers greater than this.

We could carry on with some examples more examples on this or we could go and talk about you know the curve fitting or the interpolation which also forms a very basic computational tool and is widely needed in order to understand the behaviour of a function close to a point that is important for your problem. So, one needs to fit it and there are lots of fitting algorithms and we will again see a few fitting algorithms as representative methods for these curve fitting exercise you.