Numerical Methods and Simulation
Techniques For Scientists And Engineers
Saurabh Basu
Department of Physics
Indian Institute of Technology- Guwahati

Lecture 02
Roots of Non-linear equations, Bisection Method

So, let us discuss now how errors actually propagate or rather it reduces as we take on an iterative you know method it could actually increase or decrease depending on certain situation that also we will see.

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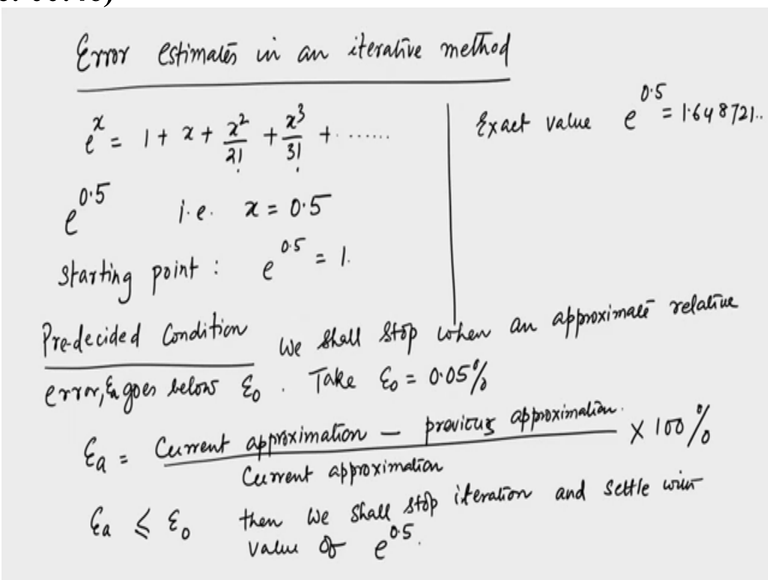

So, let us say that we talk about error estimates in an iterative method and we give you a very simple example. So, most of the mathematical functions that we come across can be expanded in terms of an infinite series. Say, for example we take this function exponential x which can be written as 1 + x + x square by 2 factorial + x cube by 3 factorial and so on. So, as we take successive terms in this expansion the value of exponential x gets better and better and it can only become exact when we take all terms up to infinity into consideration.

But since that is not possible in a numeric method we will have to truncate this series after a certain you know number of terms and your approximation or these approximation of truncating beyond a certain or rather before a certain number of terms or by a certain number of terms will make sense if the error associated with it is small and can be ignored. Let us see an example, so we want to calculate the a particular value of x say we want to calculate what is exponential 0.5 so that is you have x equal to 0.5.

Now of course we know that if we take just the first term that is like missing out a large number of terms and we get exponential of 0.5 equal to 1 which is not a good approximation. So, of course our starting point would be x equal to exponential x equal to 1 and so went .5 is equal to 1 and then we add successive terms such as x which is 0 .5 and x square by 2 factorial which is 0.5 square by 2 factorial and so on.

And then we try to see that how we converge and when we converge now the convergence will depend upon a pre-decided error that is if our successive approximation gets us below a certain error we will stop there that is the idea behind it. So, let us just you know the exact value is you can use your calculator to know that exact value. The exact value is exponential 0.5 it is equal to 1.648721 and so on, that is the exact value.

And of course we are starting with a value which is very less which is equal to 1 that is the first term in that expression and we successively add x and see what the error is compared to the exact value and we will also define a quantity called as the approximate relative error. And we will want this approximate relative error to go below a certain threshold value which will be decided by us that is by you.

So, in order to do that let us look into this that pre-decided condition we shall stop when an approximate relative error. Let me define it approximate relative error in error goes below certain number goes below epsilon 0 take epsilon 0 to be equal to .05 % that is a good enough approximation and we decide that we will stop there. If you do not think that this is a good approximation you can go even below that.

But it does not matter it will take more steps into your calculation but at this moment let us stick to this that will stop if successively computing this value of exponential 0.5. If we get to a point that our error is actually lower than this then we will stop our iteration and we will say that this is the value that we get. So, what is so this is let us call this quantity as epsilon a, so epsilon a, is defined as the current approximation and minus the previous approximation divided by the current approximation and multiply it by 10 0 in order to get it in percent.

So, that is my approximate relative error and it is also in expressed in percentage. So, if this epsilon a goes below or equal to epsilon 0 then we shall stop iteration which means including successive terms and settle with the value of exponential 0.5

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$$e^x = 1 + x = 1.5$$

$$\varepsilon_t = \frac{1.648721 - 1.5}{1.64872} \times 100\,\% = 9.62\,\%$$

$$\varepsilon_a = \frac{1.5 - 1}{1.5} \times 100\,\% = 33.3\,\%$$

Now include $\frac{x^2}{2!} = \frac{(0.5)^2}{2} = \frac{0.25}{2} = 0.125$

$e^{0.5} = 1 + 0.5 + 0.125 = 1.625 \rightarrow$ Calculate $\varepsilon_t, \varepsilon_a$.

Go to $\frac{x^3}{3!} = \frac{(0.5)^3}{6} \Rightarrow e^{0.5} = 1 + 0.5 + 0.125 + \frac{(0.5)^3}{6}.$

$\rightarrow$ Calculate $\varepsilon_t, \varepsilon_a$

So, let us see how this happens. Let us look at exponential x as 1 + x that is the first term that we are going to add and then it becomes because x equal to 0.5 then it becomes equal to 1.5. So, how far are we, so we have these or let us say now we talk about also about the truncation error or whatever the exact value minus the approximate value so that we have defined in earlier as well, so one for this is the exact value minus this approximate value divided by the exact value in 2%.

So, this becomes equal to if you calculate it becomes equal to 9.02% but even more serious error is caused at the this approximation level where this level of approximation yields 1.5 the other one yields 1, so divided by the current approximation in 20 0 that gives us a value which is thirty 3.3% so this value 1.5 is way off compared to 1.6 for and we cannot stop here. So, now include x square by 2factorial which is you know so this is 0 .5square by 2 which is equal to 0 . 25 divided by 2which is equal to 1. sorry 0 .125.

And if we actually include it then it becomes so exponential .5 at this level becomes equal to 1 + 0 .5+ 0 .125 and this becomes equal to 1.625 we are still away and we can calculate the epsilon t which is the error the percentage relative error and also the approximate relative error. And these can be calculated in person and then so calculate epsilon t and epsilon a then of course go to x cube by 3 factorial which is nothing but .5 whole cube by it is 6.

And then you add it to this term so this becomes this gives a exponential 0 .5 equal to 1 + 0 .5+ 0 .125+ this quantity I am not calculating it but you can use your calculator and can do it so at this level it is this and then again calculate epsilon t and epsilon a. Check whether epsilon a falls below.0 5% and if it does then you are done.

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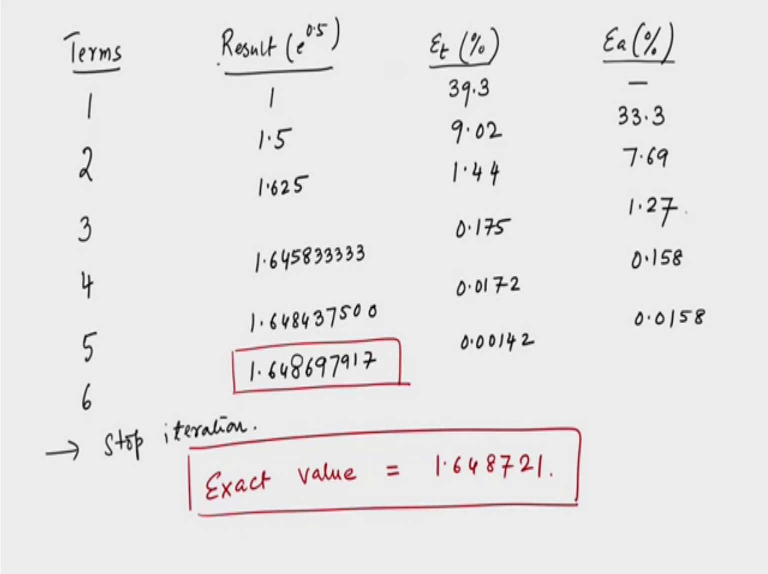

Terms	Result ($e^{0.5}$)	ε_t (%)	ε_a (%)
1	1	39.3	—
2	1.5	9.02	33.3
3	1.625	1.44	7.69
4	1.645833333	0.175	1.27
5	1.648437500	0.0172	0.158
6	$\boxed{1.648697917}$	0.00142	0.0158

→ Stop iteration.

$\boxed{\text{Exact value} = 1.648721.}$

So, let us make a table out of it and we will say that this is the terms this is the result that is what we get out of these, so it is basically result for exponential .5 by adding successive terms. And then how we have the relative error in percent in percent and this is that approximate error in percent. So, remember this epsilon t, Epsilon actually stands for error is just a convention. This is taken with respect to the exact value.

Now because we know the exact value here by a trivial you know computation using either a computer or just a even a calculator would do that is why we are calculating this, but if this is not available that is you do not know the exact value then of course the only thing that is important for us is this approximate relative error which calculates the error as it propagates or rather as it goes down in you know taking into account various terms.

So, we are actually talking about errors going down if we take more and more terms into these infinites of these infinite series into consideration. All right so your 1 if this is equal to 1 and this is 39.3% you can check that which is 1.648that number 648721 - 1 divided by 1.648721 in 2% so that comes to about 40 % and of course there is no there is no approximate error in this particular step because we are just starting this that is the first step.

And when you go to the second step then the result is 1.5 we have already computed that this is 9.0 3 and we have already computed that this is thirty 3.3 so you see the error has come down by including just 1 term from 39% to about 9% in the third iteration when you also include an x square by 2factorial which is the third term and 1 gets a 1.625 which is what we have seen we have not calculated it but you do it I suggest that you do it and this comes down drastically to 6.; 7.69% and the 4that is equal to your 1.6458 and 33333 and this is only 0 .175% and this is 1.27%.

Similarly in the fifth iteration 1 gets a 1.648437500 and 1 gets it as .0 172 and 1 gets it less than 1% error which is 0 .158, we still are above that .0 5% but maybe 1 more step could take care of it and it does in fact it gives you 1468648697917 and this is 0 .0 0 .0 0 142 and this is really .0 158 so you see that it falls below .0 5% and we can stop the iteration. stop iteration One of course good thing to ask that how the error converges.

In how many steps the error would converge to a desired value and in that case you need to know the analytic form of the convergence and that also can be found we will see an example. So, now this is a value this is the result is this is the final value that we take as and if you think about it our exact value was 1.648721. So, so that is that is fairly close it is 8697 if you take so it is 146 1.6487instead of 869 and so on.

So this is the exact value and we get within only 6 iterations this is converged to a value that is desirable in this particular context. So, this is you know there are just 2 examples that we have considered in the first example in the Rail track problem we have considered, how taking a slightly, you know lesser approach or rather very approximate expression for calculating where the rail track would be joined gave me a result which is way off than a certain slightly better approximation.

And here you see that in an infinite series as we keep adding the terms in the infinite series. You have these convergence of these values to the exact values very fast. In fact if you go to one more step you will probably get a value which is very very very very close. So, that is because already we are at the approximate error to have a value less than.0 5% in fact it is.0 1% just about that.

So, we will continue with this error as and when with every method that we actually learn and it is very important for us to know that how the errors propagate. What is the analytic form of the error and how they are going to affect our you know our calculations or rather our predictions of the physical things that we are trying to.

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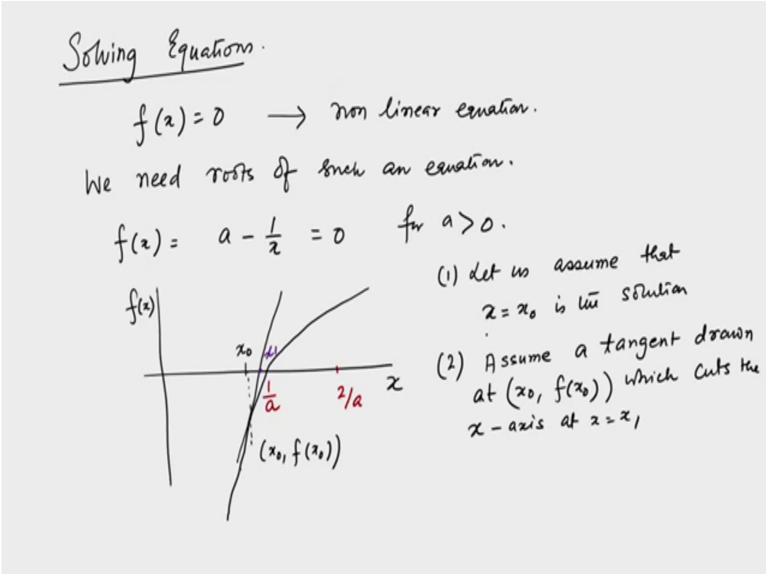

So, let us now go to a topic a particular topic of discussion which we are all familiar to right from our you know mid school days which are about solving equations. I mean these equations are there everywhere we have learned Newton's laws of motion or Newton's second law very early in our carrier and we know that it is a second order linear differential equation in the absence of any damping term and we need to solve it.

And sometimes these equations are differential equations sometimes these equations are simply algebraic equations with just one unknown. And sometimes there are more complicated equations which are systems of equations with more than one unknown and sometimes large number of unknowns. And analytically it becomes a problem to solve anything with more than 2 or 3unknowns. And even sometimes 3 unknowns become a problem unless we are given another condition in some physical situations that may arise.

And we are you know interested in talking about solutions of equations but these equations are mostly nonlinear equations. Linear equations I believe that these are easier to solve nonlinear equations are more difficult and sometimes the non-linearity is quite complicated and we need to get to the fact that we have to sometimes solve nonlinear equations and those nonlinear equations there should be some numerical methods to solve those nonlinear equations.

So, any equation is cast in the form f of x equal to 0, I mean that is the we need to solve say there is a nonlinear equation and we need the roots of that. So, take an example that let us say one has to solve a F x equal to a - 1 over x which is equal to 0 for a to be greater than 0 way simple equation you do not want does not really need a numerical method to do that x is equal to 1 over a is the solution everybody knows.

But suppose it is not a simple equation as simple as this but it is a complicated equation but can we talk about a genetic method or a general method in order to address such complicated more complicated nonlinear equation. Let us see that so of course if I you know plot this thing it will look like so this is f of x as a function of x and if I do it, it looks like this and it has a crossing at let us show it by a different colour at 1 over a.

So, at 1 over a there is a point the crossing point and say this is 2 over a and things like that and then of course that is there and but we do not know the solution of this that is the assumption of course. We know here but let us assume that we do not know the solution. And if we do not know the solution let us take a solution, let us assume that x equal to x0 is the solution which means I do not know exactly where it is but I assume that it is somewhere here is the solution I just guessed it.

Nobody told me it could be a wild guess I could have guessed it somewhere far away on the x-axis but then I would have you know there are problems with that which we are going to see in a while. But say we have somehow guessed it approximately correct and it is not too far away from 1 over a and this x0 lies in the somewhere in the vicinity of that. Now what we do is that we take this point which is called a point x0 fx0 that is the xy point and draw tangent at this point.

I have to be careful, it is not touching, so let me, I mean, I want to draw a tangent at this point let me just draw both the curves a little better. So, I have this curve which is like this and my at x0 I want to draw tangent ok. I did a tangent ok approximately take that as a tangent slightly harder to draw on this board. But that is the tangent so I drew a tangent at this point so this is step number 1 this is step number 2 that assume a tangent drawn at x0 and fx0 which cuts the x-axis at x equal to x1.

So x1 let me write it with a different colour this x1 this point, x1 which is this point ok, so this point x1 is my new root of this equation fx equal to a - 1 over x and which is a better approximation than the x0 that I have all originally assumed. Now you could say that I could have assumed very wrong point where the tangent cannot be drawn or the function has you know you cannot either draw tangent there or there is something that is wrong with this.

And we could actually go away from x0 so x0 could have been a better estimate than x1 that could happen I'm not denying the fact. So, there are certain conditions which you have to obey or which you have to follow in order to find or guess a root of this equation in a slightly you know intelligent manner all right. So, this is the this is the situation so we have drawn this and we have got a point x1 which is the solution ok.

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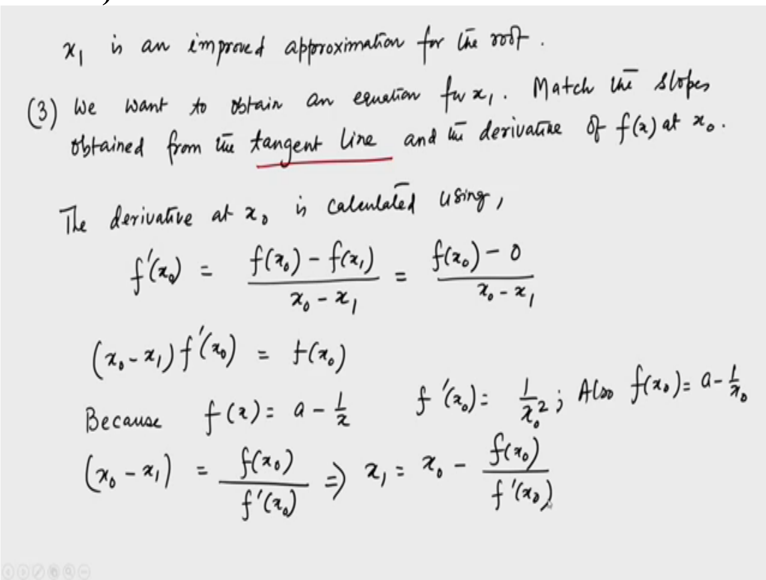

So, x1 is an improved approximation for for the route now number 3 we want to obtain an equation for x1 such that solving it I get a value of x1 and in terms of x0 which is your original guess and if we can form an induction or rather by induction if we can say that you know the same equation is actually it the same equation also describes x2 starting from a value x1 which was our previous guess.

So, if that is possible then of course you form an iterative you know equation which successively one solves the 1 gets a x1 x2 x3 x4 and successively you make the root better and better. So, in order to do this match the slopes obtained from the tangent line from the tangent line and and the derivative of fx at x0. I mean they are same so I am just matching them or rather equating them.

So, the derivative at x or x0 is calculated using f prime of x equal to f of x0 - f of x1 is just a 2 point derivative which we will learn in a more detailed manner as the course progresses. And so this is a 2 point method by which we take the derivative between 2 neighbouring points calculate the value of the function and the neighbouring points and take the difference between the 2 points and f of x0 - 0 because F of x1 is equal to 0.

If you see the function the function actually has a value 0 at x1 equal to 0 because it touches the you know the x axis. And this is nothing but x0 - x1 correct. So, this is fine now I just do a cross multiplication of this so it is x0 - x1 F prime of x this is equal to f of x0. Now you see from because; my because I have f of x equal to a - 1 over x, I can calculate F prime of x is equal to 1 over x square and what is my f of x you also f of x0 is equal to a - 1 over x0. So, these are the 2 things that are there so I am just going to put though them just before that let us finish 1 more step.

So, it is f of x0 divided by F prime of x and this gives me x1 equal to x0 - f of x0 and so this is this is actually a calculate; this is the; the thing is calculated the slope is calculated at x equal to x0. So, this is actually x0 and this is also at x0, so this is x0, so this is x0 and so on. So, this is f prime of x0 and this is nothing but;

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$$x_1 = x_0 - \frac{a - \frac{1}{x_0}}{\frac{1}{x_0^2}} = x_0 - x_0^2\left(a - \frac{1}{x_0}\right) = x_0 - a x_0^2 + x_0.$$

$$\boxed{x_1 = x_0 (2 - a x_0)}$$

A general iteration method can be used,

$$x_{n+1} = x_n (2 - a x_n) \qquad n \geq 0.$$

Use a slight change in variable, $r_n = 1 - a x_n \Rightarrow \frac{r_n}{a} = \frac{1}{a} - x_n$

$$x_{n+1} = x_n(1 + \underbrace{1 - a x_n}_{r_n}) = x_n (1 + r_n).$$

Error $\varepsilon_n = \frac{1}{a} - x_n = \frac{r_n}{a}$

So, we got a relationship for x1 in terms of x0 and remember this is what is wanted or rather this is what was desirable to begin with that we get the value of this new root and find a relationship with it the old root and the old root in this case is a starting value. So, my x equal or rather x1 equal to a - 1 by x0 divided by 1 by x0 square so this is f of x0 the numerator is f of x0 and then it is f prime of x0 and so this is sorry there is a x0 that is missing and it is this ok.

And if you simplify this, this becomes equal to x0 - x0 square a by 1 - x0 and this is equal to x0 - a x0 square + x0 and this if you simplify then it becomes x1 becomes equal to x0 2 - a x0. So, this of course gives me an equation of x1 in terms of x0 and this is something that is you know is important for us, let us see this carefully. So, a general iteration method can be used because we have started with only a pair of values of x1 and x0.

So, we can take it rather continue it for any xn + 1 and xn and so this is xn + 1 which is the new approximate root – 2 - a into the old root and for n of course greater than equal to 0. Use a slight change in variable then we have if we write r n this is equal to 1 - ax n then we can write xn + 1 equal to xn 1 + 1 - ax n and this is nothing but r n, so this is equal to xn 1 + r n and the error is in this case is equal to epsilon n let us call it epsilon n at the nth level which is equal to 1 over a - x to the power n at the nth level.

This is the exact root we are not talking about the relative 1 and as yet it is just the just a bear you know error which is the exact value - the approximate value at the nth iteration. Now if that is true then this is nothing but equal to r n divided by a see the r n has a definition so this gives you r n by a, r n by a equal to 1 over a - xn and since we have 1 over a - xn here so this is equal to r n over a. So, that is the error at the nth level.

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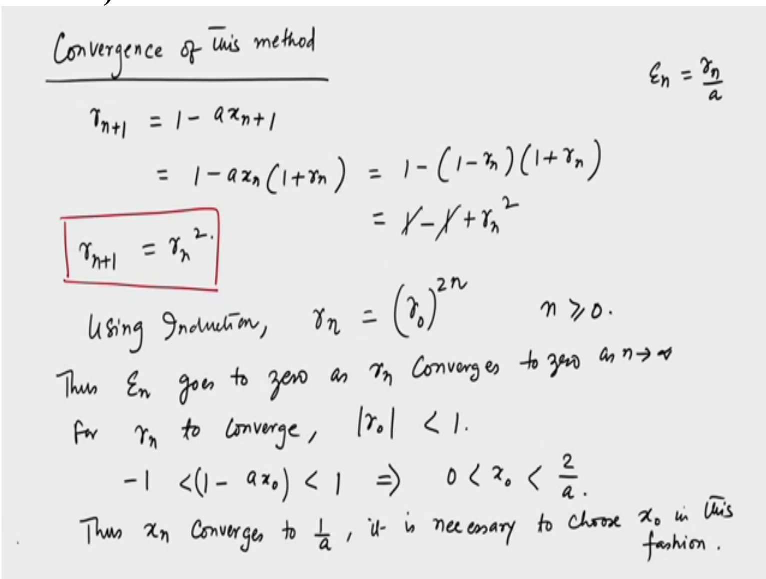

And now we want to check the convergence of this method. So, the convergence of this method is can be tested as follows so it is r n + 1 which is equal to 1 - ax n + 1 and this is the definition of rn because we started from rn equal to 1 - ax and so rn + 1 is equal to 1 – ax n + 1 and if you look at the definition of ax n I mean just xn + 1 here this is the definition xn + 1 it is equal to xn 1 + rn and so we can write this as 1 - ax n 1 + rn.

And this is nothing but equal to 1 - 1rn + 1 + rn because ax n is nothing but 1 – rn, so that gives if you simplify this basically what you need to do is that you just open the bracket so this is equal to + it is a + rn square so this will cancel so I what I get is that rn + 1 is equal to rn square. So, this is an important thing result that we have that using induction again 1 can get our n equal to r0 to the power 2n ok.

So, if you put n equal to 0 then I get r1 as R 0 square and then use for r2putting n equal to 2I will get R 3equal to r2 square but r2 is nothing but r1 square so you gather a square at every stage so at the nth stage you gather a factor of 2n in the power and this is your the rn this thing and of course as I said earlier that n is greater than equal to 0. So, this E n goes to 0 as rn converges to 0, 0 as n tends to infinity.

Remember what is the relation the relation is that that your epsilon n is nothing but r n by a and a is greater than 0, so r n epsilon n will go to 0 if r n goes to 0 as n goes to infinity it should not grow it should you know die down so for that to happen so for r n for r n to converge we need r0 less than 1 so the mod of r0 should be less than 1 so that is how it has to be chosen let us go through 1 more step and then it will be clearer to you.

So, a - 1 less than 1 - a x0 less than 1 so you see this are 0 because the definition of r0 is 1 - ax0 so a 1 - ax0 should lie between a - 1 and + 1 for the convergence to occur. So, this of course gives the condition that 0 is less than x0 is less than 2- 2by a so in this particular situation let us go back to this original figure. If your x0 does not satisfy that condition that is between 0 and 0 is here and to buy a that is why we have plotted to buy a then you have no chance of converging does not matter how many steps you follow in this iterative scheme to reach closer and closer to the exact solution.

So, that is the condition and we said that it is not any value that would do it you have to have an intelligent value and the value comes out that it should be between 0 and 2by a which is shown in that plot that I just showed you. Thus xn converges to 1 over a it is necessary to choose x0 in I mean constrained by this or rather in this fashion whatever you want to write. So, that is the condition for 1 to have a convergence and so on and let us see the nature of convergence this is what I was saying earlier that we need to understand that how the converges happens.
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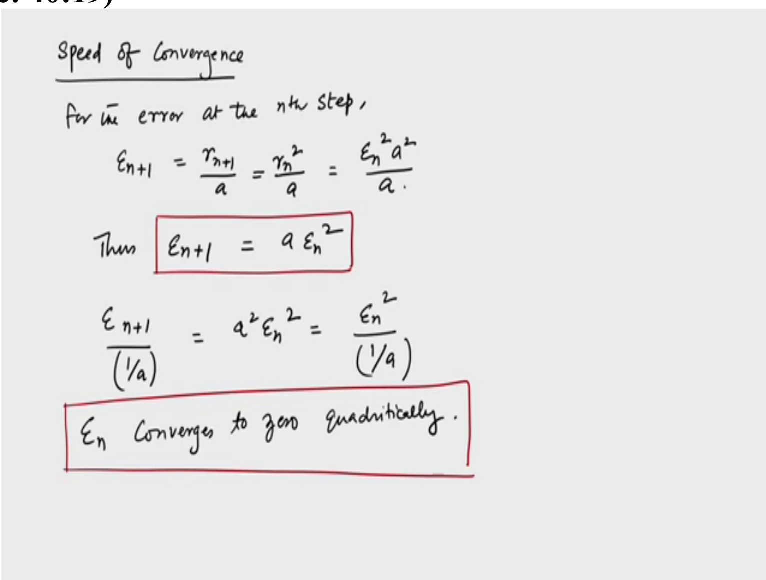

So, let us talk about the let us say pace or speed of convergence. So, for the error at the nth step E n + 1 equal to r n + by n + 1 by a which is nothing but our n square by a which is equal to E n square a square by a, so that is the convergence that is epsilon the error at the n + 1 at level varies as a square of the error at the n at level, so of course if epsilon n is small in successive steps it gets smaller and smaller and this is what we have seen in that last problem that we did.

Thus epsilon n + 1 is simply a epsilon n square this is the convergence and in any iterative method we should test the convergence. So, we can simply write this as epsilon n + 1 it does not matter of course I mean it is 1 over a this is equal to a square epsilon n square which is equal to epsilon n square divided by 1 by a square and so on. So, what what I trying to say is that the epsilon n converges to 0 quadratically.

And that is the speed of convergence if you want faster convergence that is power which is larger than 2 then there has to be you know different method in order to implement this and so on. In a root finding problem usually we find that these are convergent in this particular fashion that is a quadratic convergence. And quadratic convergence is good because if you are you know usually in normal nonlinear equations that we come across the convergence is quite fast in fact in does not have to go to too many iterations in order to have convergence of this.

So, thus we have what we have done is that we have taken a problem of non-linear equation it of course the interpretation goes to you I have taken a very simple equation 1 over a equal to x or 1 over f of x equal to 1 over a - x equal to 0 that equation had to be solved. And what we did is that we have taken a guess value x0 calculated the slope of the value at x0 fx0 that is xy point. And extended that tangent to meet the x axis so that we know the new position of the new root and then we have found out in induction formula that how we can actually iterate the roots from 1 approximation or 1 you know iterate iteration step to another.

And this is how we have gone ahead and converged the convergence comes out to be a quadratic convergence ok. So, we will see some examples related to that.