Numerical Methods and Simulation
Techniques For Scientists And Engineers
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Lecture 03
Newton Raphson method, Secant method

So, we are going to study the solutions of nonlinear equations in particular but it could be for any equations we will show with simple examples where we solve equations. And mainly we are going to talk about 2 methods but as an extension of these the first method that is called as bisection method will also talk about a secant method.

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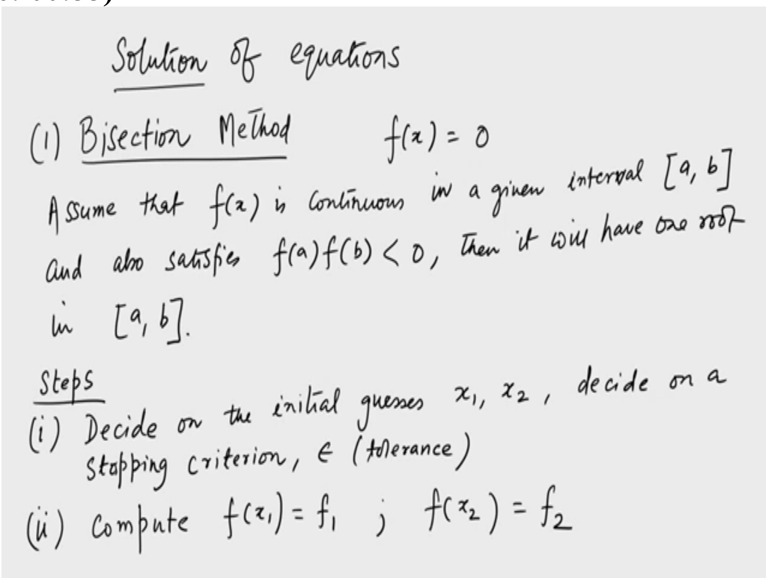

So, let us start with solution of equations and the first 1 that we discussed is called as the bisection method. It is extremely easy to understand and of course it has its difficulties and shortcomings that will also discuss. So, what is a bisection method? So, it is if you assume that you have to solve an equation which is fx equal to 0 where it has several powers of x or there are you know nonlinearities involved.

So, assume that fx is continuous on a given interval let us write in a given interval in a given interval a b that is the interval in which it is continuous it does not have any discontinuity. And it also satisfies fa into fb to be less than 0 then it will have 1 root in the interval ab okay. So, that is the condition of bisection. So, what we have to do is that we will have to start with 2 guesses for the root of an equation for which we want to I mean the equation that we want to solve.

And once we have these 2 guesses we have to calculate the functions the value of the functions at these 2 guess values and check whether the product is negative because then only the root is contained the actual root is contained within these 2 values that we have taken. So, if we really go into various steps or which you can call as algorithm as well. So, the steps are as follows. So, step number 1 it says that decide on the initial guesses and I am just calling it as x1 and x2 but it could be a and b if you like.

So, let us decide 2 guesses they could be wild guesses and you may not actually have the root subtended within that but that will be apparent once when you and you know sort of look at other conditions. Now, as I told that also decide on a on a stopping criterion which means that you would decide that whether you have reached the root by assuming a tolerance which is a number that will be decided by you.

And this number will tell you that if you have gotten a value of the root and in 2 successive iterations of these according to the bisection method. According to the algorithm that we are going to describe your the values the new values do not change or it comes within this tolerance then you say that the root is reached and that is the final answer for you problem. So, the second thing is of course which is what we said earlier that compute f of x1 call it as f1 and f of x2 call it as f2 at these 2 guess values, value of the function.

Because you have f of x so you have x1, x equal to x1 and x equal to x2 you calculate the value of the function.

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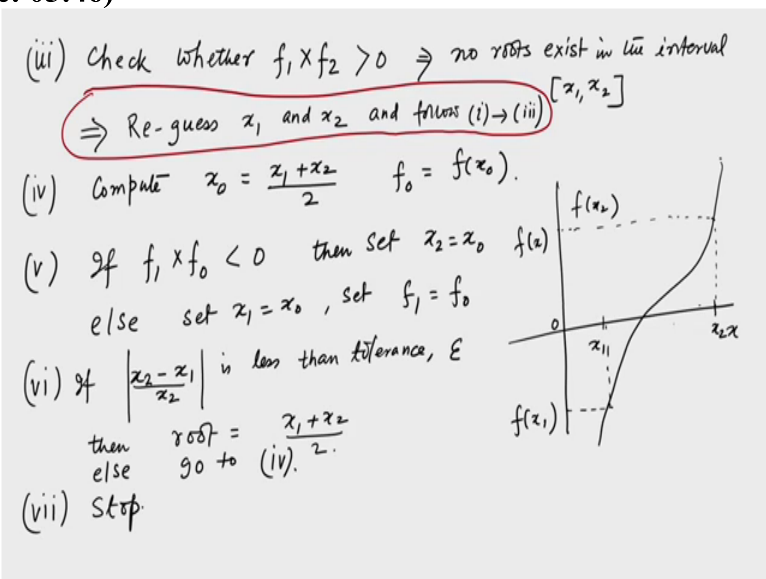

And then of course as I told that if the root is subtended then the product of these 2 values, values of the functions at x1 and x2 would give me a negative result negative result means the value less than 0 okay. So, check whether f1 multiplied by f2 is less than 0 or greater than 0 if it is greater than 0 then no roots are obtained so no roots exist in the interval x1 x2. So, which means that Re-guess x1 and x2 and follow procedure and follow 1 2 3 ok.

Now suppose the other thing happens which is what is important for us that; so these things and so on and then of course you have you can compute the midpoint that is why it is called as a bisection method. Compute the midpoint of this x1 and x2 divided by 2 and call f0 equal to f of x0 ok. So, you compute the midpoint of these things. Now look at this that now if f1 and f0 is or rather one can actually either go back to this step 1 and recalculate or rather guess it again x1 and x2 or else you can also tell this thing so we will put it in you can also follow these number 4.

So, this of course can be this is one option and the other option is of course you compute this and so on and then you follow this procedure. Now, if f1 and f2 is less than 0 suppose it does and if it does not then you have to again follow this same thing will tell you why f1 into f0 is we are checking it that it is becomes negative. Then set x2 equal to x0 ok, so this is quite important else set if this does not does not happen that is if it is not less than 0 then you set x1 equal to x0.

And set f1 equal to f0 okay so what is happening is the following if you look at this suppose this has this is the f of f of x ok versus x it has of course a crossing at this. So, now I am taking 2 values x1 and x2 and so this is my you know so this is the value of so this is my f of x2 and similarly this is my f of x1, so you see that f of x1 is of course 0, f of x1 is negative and f of x2 is positive so my actual root is subtended between, so if my root is subtended between the 2 guess values.

Then the values of the functions or the product of the values of these function would come out to be negative. And if it is not negative if I take both the points in the same direction then of course I will have both these points are in the same side of this root then of course I will get a positive value. So, suppose I take these 2 at the guest values instead of this I take this as x1 then my x1 and x2 would have a value which is here and hence it will give me a positive value f of x1 into f of x2 will be positive.

And I am not subtending the root so that is a test for whether I am subtending the root okay. So, having said that so check whether if x1 rather x2 or it does not matter actually x2 - x1 and I put a mod that is the absolute value of this divided by x2. So, this is the absolute value is less than tolerance epsilon which is already pre decided by you. Then the root is of course x1 + x2 divided by 2 and then of course you can write the root and go to 7 which is stop.

And else you go to 4 okay. So, that is the algorithm so we are a very simple algorithm that you have to choose 2 values which should subtend the root if it does not then of course you have to follow this procedure from 4 to 7 once again and if it does not follow then you have to again follow 4 to 7 or you can you know go back at the beginning and say that let me reconsider my guesses altogether and start the procedure all over again.

Nevertheless both are same and it is an easy as I said it is an easy method however it has shortcomings that is the convergence rate is slow and let us show that.

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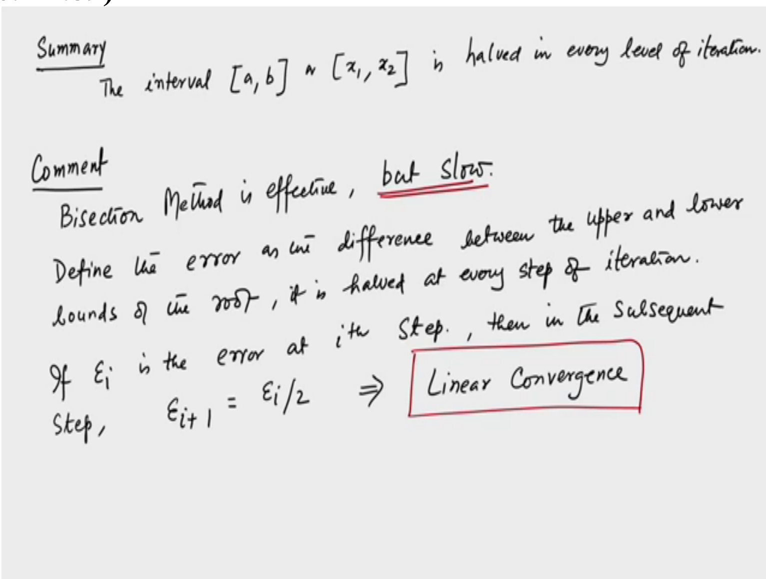

So, the basic summary if you like the interval ab or x1, x2 as has been taken in this particular problem is haft in every level of iteration. So, it is every time we are restricting the value or we are trying to find the root but by coming by making that interval to be half every time and that is why we are trying to 0 in on the root and getting when we actually have 2 values which fall below the tolerance then we claim that the root is achieved okay.

So, it is basically the comment is that it is bisection method is effective but slow and we want to highlight this why, is it slow. So, if you define the error as the difference between the upper and lower bounds of the root it is halved so the error is halved every time at every step of iteration thus if epsilon i is the error at the ith step then in the subsequent step, that is epsilon i + 1 is simply equal to epsilon i by 2.

So, this says that it has a linear convergence so that is why it is slow and it sort of gives you root even if it gives you sort of finally it gives you the root the steps the number of steps that you have to follow in your computer is quite may be quite large depending on situation okay.

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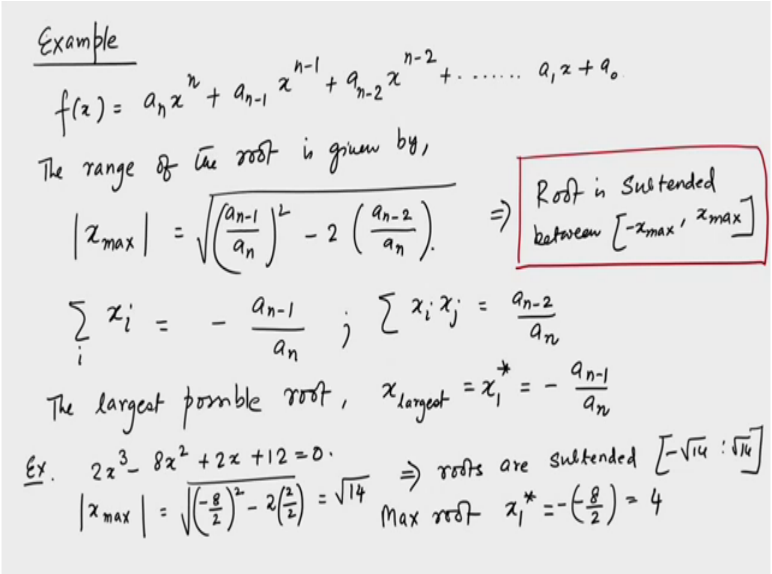

So, let us see an example simple example let us write down a polynomial, so polynomial f of x is written as a n x n + a n - 1 x to the power n - 1 + a n - 2 x to the power n - 2 and + this and then I have a 1 x + a 0 that is a nth degree polynomial in that we have and we can try to solve this equation that is put f of x equal to 0 and then solve for the you know the particular root that we are interested.

In the range of the root it is important to know this mathematical formula the range of the root is given by these coefficients there is so let us call it x max and a mod this is equal to root over a n - 1 divided by a n whole square that is the coefficient of the second term the sub leading term and divided by the leading term that - 2 and another lower than that and then this and so on. So, that is the formula for the range of the root.

So, the root is subtended between - x max to + x max so this tells that the root is subtended and it is an important thing. So, this comes from basic equations for polynomial equations solution of equations and so on. So, basically there are some other results which could also be important so let me write them that the sum of the roots which is x i sum over i that is the sum of the roots is equal to - a n - 1 divided by a n and the product of the roots which is x i x j that is equal to a n by a n okay.

So, that these things are known from your school days that this is how so this is the sum of the all the roots is equal to negative of minus this that sub leading term the next term are divided by the leading term and the product of the root that involves the coefficient of the next term divided by the leading term. So, basically the largest possible root, so this possible of course because you know that it is x subtended between - x max to + x max.

But suppose all other roots are 0 only 1 root survived then of course this is given by let us call that as x large largest call it by x star and that is equal to - a n - 1 divided by a n because the sum of all the roots is this so if a 1 root only 1 root exists let us write it as then x1 just that to signify that 1 root exists. Then that is that will also be given by this ratio the coefficients. So, these are something that are unknown to you.

Let us take an example let us take this example of 2 x cube - 8 x square + 2 x + 12 equal to 0 the x max here this is equal to - 8 divided by 2 whole square - 2 into 2 by 2, so this is equal to root 14, so this tells that roots are subtended in the interval - root 14 to 14. So, bisection necessarily asks you or to guess the 2 values where the term that the actual root is subtended. So, now you get a idea get an idea that how the values could be chosen or they could be guessed such that you have these roots that are subtended there.

And of course so the roots must lie between this and so on and of course if you like the maximum root which is x1 star is simply equal to you know - 8 by 2 - of - 8 by 2 which is equal to 4, so the largest root is 4, so we can also take it instead of root 14 we can also go to + 4 and – 4. But as you see that root 14 is less than 4, so you have a tighter interval anyway here. And it makes sense because not all the other roots would be 0 because this maximum root assumes a formula where all the other roots would be 0 and only 1 root exists.

So, either you can take it from - 4 to + 4 or you can take it from - root 14 - + root 14 well it makes more sense to take it from - root 14 - + root 14 okay.

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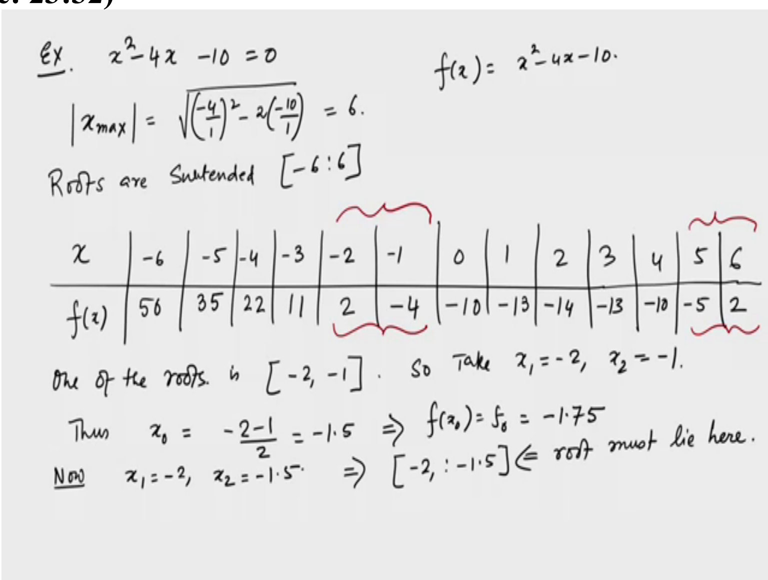

So, let us take a sort of concrete example in order to do that so let us take x square - 4x - 10 equal to 0. Now please remember that some of these problems that we do here are can be solved either by hand or by using you know the simplest software package that you have. But it is we have taken those for the sake of demonstrating the property or the power of these methods that we want to show okay. So, the examples are quite light and if you say very simple but they nevertheless show the utility of the method.

So, this is a simple quadratic equation you could have solved it without much problem but now we do it using this bisection method. And of course what is my x max here in order to get the idea of the root that is equal to root over - 4 + - 4 by 1 square - 2 into - 10 by 1 and this is equal to 6 so roots are subtended in the interval – 6 to + 6 okay so that is the interval that it is subtended in.

Now let us calculate the value of the function and so let me make a table that so these are x and f of x and make several let us see whether we need to go so it is a – 6 - 5 we need many more - 4 - 3 - 2 - 1 0 1 2 3 4 5 and 6 ok, so the value of the function that is x square - so f of x is equal to x square - 4x – 10, so at x equal to - 6 we have a value 50 because it is 36 + 24 – 10, so 36 + 24 becomes 60, 60 - 10 becomes 50 and then at this thing it becomes 35 and then it becomes you know 22.

Why I am doing that is that I want to see where it changes sign because then I will understand where the roots are subtended and 11 for - 3 and for 2 and then from - 1 it becomes - 4 for 0 it becomes -10 for 1 it becomes –13 -14 again becomes -13 -10 and -5 and 2 you can check these things carefully. So, it becomes 36 for the last value it becomes 36 - 24 -10 so 24 + 10 34 36 - and 34 is equal to 2, so these are the values that we have.

So, what is important for us is this interval, so roots must be subtended within this ok so that that is the part which is important for this discussion, root is or at least 1 root let us call it as 1 root 1 of the roots and of course the other root could be there also I mean there is a 0 crossing here as well and so on, is in the interval - 2 -1 okay. In this interval and so take x2 or x1 equal to - 2 and x2 equal to – 1.

So, what is x0 because we have to have that interval we already know what is f of x1 into f of x2 which are these 2 values and the product comes out to be negative so we straight away if you like we are going to this fourth stage because we have already checked till stage number 3 or step number 3, x0 is equal to - 1 - 2 by 2 which is equal to – 1.5 that gives me f of x 0 which is equal to f 0 its equal to -1.75 you see f0 is - 1.75 because we have calculated this f of x at x equal to 1.5, - 1.5.

Now you see that this has a negative value and so is the value at f equal to - 1 x equal to - 1 f of x at x equal to - 1 as a negative value. So, it is now subtended between 2 and -1.5 okay so I take this value as the new guessed value for x, x2 I take this as a new guessed value for x2, so my x1 remains as - 2 and now if you like in the next step your x1 remains as - 2 x2 no longer remains as - 1 and but because it but it becomes equal to - 1.5, because of the reason that I told that you see that there is this is 2 which is positive and this is – 1.75 which is negative.

So, the sign change must be occurring here so the root must be extend subtended between these - 2 and -1.5 so root must lie here one of the roots as I said.

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In the next step,

$x_1 = -2, \quad x_2 = -1.5, \quad x_0 = \frac{x_1 + x_2}{2} = -1.75$

$f(x_0) = f(-1.75) = 0.0625$

Root is <u>not</u> subtended $[-2 : -1.75]$ but rather in $[-1.75 : -1.5]$

$x_0 = -1.625 \Rightarrow$ Calculate $f(x_0)$

Proceed similarly.

$\boxed{\text{Approximate root} = -1.7416.}$

So, in the next step x1 equal to – 2, x2 equal to -1.5, x0 that is which is x1 + x2 divided by 2 becomes -1.75 and calculate at this new midpoint and this is equal to –1.75 which becomes equal to - 0 in + 0.; I am so sorry it is 0.0625 please check all these numbers as you practice these problems. Now you see your f of 2 is positive f of - 1.75 is also positive which means the root is not subtended between 2 and – 1.75 rather it is subtended between -1.75 and – 1.5 because both of them give different signs for the value of the values of the functions.

So, this is there so I root is not subtended in the interval – 2, -1.75 but rather in - 1.75, - 1.5 so new x0 becomes equal to – 1.625 and so on ok. So, please proceed with this so calculate f of x0 see whether it has a sign that is same as – 1.75 or – 1.5 then sorry see whether it has the same sign yeah with either of these values if it has the same sign with - 1.5 then the root is subtended between – 1.625 and – 1.5 find the midpoint calculate the value of the function at the midpoint and this thing.

And if you actually do it like this then the let us write proceed similarly and if you proceed similarly the approximate root I am giving you the result with some tolerance is it could be its – 1.7416 you have you can have a accuracy of 10 to the power -3 or 10 to the power -4 or that is completely up to you that how we accurately you want to have the root but this is the solution of that problem using bisection method.

So this is the problem x square - 4x - 10 equal to 0 and the numerically 1 can find that the approximate root is this alright. This is the bisection method as I told that it is it is very easy as well as very sort of under having a slow convergence. Now so far you are to look for 2 roots and they should subtend the actual root which is checked by seeing the value of the functions whether it changes sign between these intervals.

But suppose you want to do it with any 2 guesses is that possible and that is possible using a method called a secant method.

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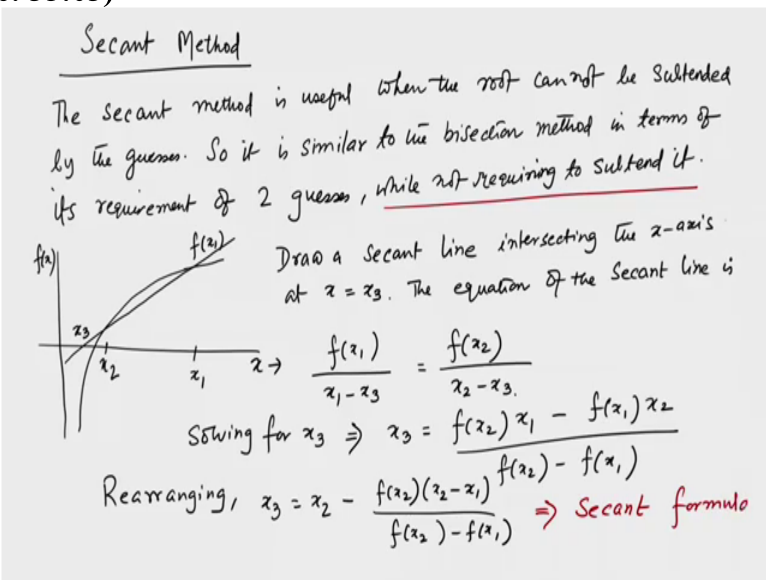

So, the secant method is useful when the root cannot be subtended or the guess you can take any 2 guesses. So, what happens when you take a guess which is not good guess then of course you have to resort to a different method. It still requires you to guess 2 values for the roots nevertheless. So, that way it is similar to the bisection method in terms of its requirement of 2 guesses while not requiring subtending it so this is this part is important okay.

So, let me draw this figure so we take 2 values x1 and x2 both in the same side of the root that is not subtending the root. And draw so this point, so draw a secant so you calculate so calculate f x1 sorry and this has to be so let me shift the x2 because it has to cross at x2 just a moment, so your x2 is here, okay and this is let us call it as x3, this is f of x and so on okay. So, that is so draw a secant line intersecting the x-axis at x equal to x3.

So, the equation of the second line is f of x1 x1 - x3 equal to f of x2 x2 - x3 so 1 can solve for x3 which is on the other side of the root x3 equal to f of x2 multiplied by x1 - f of x1 multiplied by x2 divided by f of x2 - f of x1 that is a value of x3 from this equation. So, if you rearrange then one gets x3 equal to x2 - f of x2 x2 - x1 divided by f of x2 - f of x1 okay that is the value of x3 so that is the equation for x3 in terms of x1 and x2.

Remember x1 and x2 are the 2 guesses that we have taken and just for the sake of demonstrating this as if we have intentionally taken them to lie on 1 side of the root so this is called as the secant formula now of course the important thing lies not in the method but a how it is superior to the bisection method. Of course one thing is that if you do not know the position of the root you might actually be misled in trying to guess it on either side of the of the actual root.

So you might actually land up guessing in same side of the root but that is one advantage of the secant method that it does not require you to guess it add on both sides of the actual root. But also more than that there is a convergence thing that is important here. Of course we have seen that in bisection method the convergence is linear that is every step the error is reduced to half. So, if the error is epsilon i at a given stage at epsilon i + 1 it is I mean i + 1 it is step epsilon i + 1 will simply be half of epsilon i that is epsilon i by 2. Now whether the second formula has any other convergence rate is what one needs to see.

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Convergence of the Secant Method

Secant formula for iteration,

$$x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})} \qquad (1)$$

Let x_r is the actual root of $f(x)$ and ϵ_i is the error in estimating x_i.

$$x_{i+1} = \epsilon_{i+1} + x_r$$
$$x_i = \epsilon_i + x_r$$
$$x_{i-1} = \epsilon_{i-1} + x_r$$

So, let us just talk about the convergence of the secant method. So, let us write down the secant formula once again which we have written in the last slide for iteration now. So, it is i + 1 has to be equal to x i - f of x i x i – x i - 1 divided by f of x i - f of x i - 1 so just to remind you that it was x3 which is the value that is here is equal to x2. So. if this is the you know the level of iteration that we are talking about so it is x2 so is x2 and then fx2 - f of x2 and then x2 - x1 and so on.

So, that is written simply as x i + 1 is equal to x i and then f of x i and x i x i - 1 and so on ok. So, that is the equation or rather that is the secant formula. So, let x r be the actual root of f of x and epsilon i is the error in estimating x i, x i + 1 equal to epsilon i + 1 + x r, so that is the understanding that at the i + 1 at level it is the error is epsilon i + 1 and that is the real value. So, you are off from the real value by this amount which is epsilon i + 1.

Similarly x i, so let us call this as equation number 1 this is equal to epsilon i + x r and x i - 1 which is related to that you know x1 and x2 and so on its epsilon i - 1 + x r so each 1 of them is off from the real value by these respective errors which are epsilon i + 1 epsilon i and epsilon i - 1 so let us call this as equation 2.

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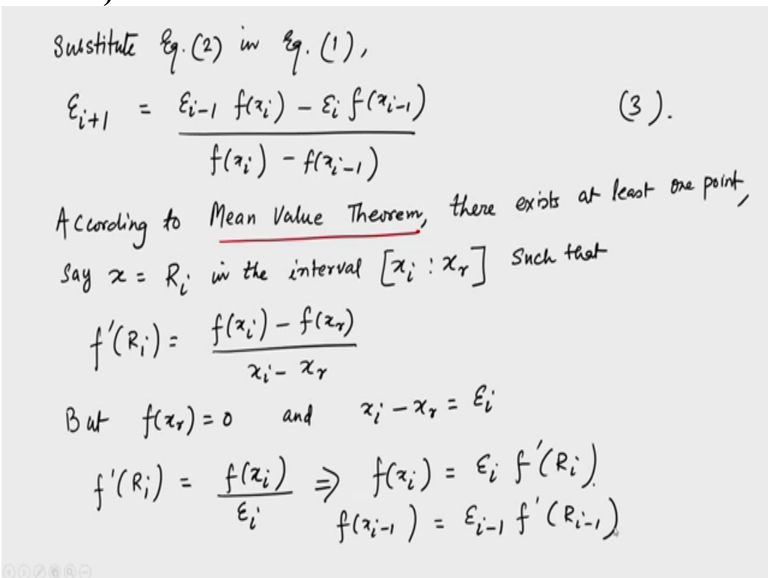

If you substitute equation 2 in equation 1 then epsilon i + 1 it is equal to epsilon i - 1 f of x i - epsilon i f of x i - 1 divided by of course f of x i - f of x i - 1 that is called equation number 3 that is the value of the error at the i + 1 at step. So, just reminding you that we are trying to look for the convergence speed of a secant method and if it is any different than linear convergence that we have already seen for the bisection method.

So, now I will invoke result which is you can look at any mathematics book or probability and statistics book and so on. And so we invoke what is called as a mean value theorem so please read about it. So, we will simply state and go but you should once have a look at it. According to mean value theorem there exists at least one point this is the mean value theorem. So, there exists one point so the mean value theorem is about the continuity of a function and its first partial derivatives.

So, if you have you know 2 functions in the vicinity let us call them as p and q then the straight line joining p and q if it fully lies in a given domain d then of course they are the difference between these functions at these neighbouring points can be expressed as a the first partial derivatives of these points evaluated at the points I mean evaluated at these points in d. I am not going into details but please have a look at it once.

So, I am using the result that there exists at least one point say x equal to say x equal to R i in the interval this is a physical interval that we are talking about x i and x r where r as I told r is a real root. So, there has to be at least one point let us call that point as x equal to R i in this interval such that the derivative f prime R i it is equal to f of x i- f of x r divided by x i - x r this is precisely the statement of the mean value theorem.

But of course f of x r is equal to 0 because that is the real root so x r is equal to 0 and for our case x i - x r as has been postulated here just above in the last slide that is from this equation second of the equation 2 so x i - x r equal to epsilon i, now f prime of R i will just put these all these 2 information into this, so this is equal to f of x i divided by epsilon i that gives me an equation which is f of x i that is a value of the function of the ith equation it is equal to epsilon i f prime of R i.

And so f of x i - 1 that is equal to epsilon i - 1 and f R i - 1 which all these values relate to the i actually index refers to the iteration step.

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Substitute (4) in the numerator of 3,

$$\epsilon_{i+1} = \epsilon_i \epsilon_{i-1}\left(\frac{f'(R_i) - f'(R_{i-1})}{f(x_i) - f(x_{i-1})}\right)$$

$$\boxed{\epsilon_{i+1} \propto \epsilon_i \epsilon_{i-1}}$$

Now the order of convergence of an iteration process is p, if

$$\epsilon_{i+1} \propto \epsilon_i^p$$

Thus, $\epsilon_i^p \propto \epsilon_{i-1}^p \epsilon_{i-1}$

$$\epsilon_i \propto \epsilon_{i-1}^{(p+1)/p}.$$

$\Rightarrow$ Since $\epsilon_{i+1} \propto \epsilon_i \epsilon_{i+1}$

Alright so far so good we have let us call this as equation 4 and if you substitute 4 in 3 substitute 4 in the numerator of 3 epsilon i + 1 equal to epsilon i epsilon i - 1 f prime of R i - f prime of R i - 1 divided by f of x i - f of x i - 1 ok this is how the error at the i + 1th at level appear. Now, these are values ok so these ones that I keep it in bracket now are values so epsilon i + 1 is proportional to the product of epsilon i and epsilon i – 1.

So, this is an important result that we get ok now let us now the order of convergence of an iteration mechanism or iteration process is p if epsilon i + 1 epsilon i + 1 is proportional to epsilon i to the power p, so this is the order of convergence of an iteration process if it is p then if epsilon i + 1 goes as epsilon i to the power p then the convergence is of this particular process is p. So, then epsilon i to the power p as or rather epsilon i to the power p is proportional to epsilon i - 1 to the power p and epsilon i – 1.

So which means that epsilon i is proportional to epsilon i - 1 and a p + 1 divided by p, so this is how the this happens of course because of this is because your epsilon i + 1 since is proportional to the epsilon i epsilon i + 1.

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$$p = (p+1)/p$$

$$\Rightarrow p^2 = p+1 \Rightarrow p^2 - p - 1 = 0.$$

$$\Rightarrow p = \frac{1 \pm \sqrt{5}}{2} = 1.618 \text{ (for positive sign).}$$

Secant Method has a super linear convergence.

Since $1.618 > 1$, $\boxed{\text{Secant Method has faster Convergence than the bisection method.}}$

So, which means that p is equal to p + 1 by p + 1 by p and that tells you that p square equal to p + 1, so we have to solve a p square - p - 1 equal to 0 that gives a solution p equal to 1 + - root over root 5 by 2 and this is equal to 1.618 of course if I take the further positive root that is a larger root for the; so what it says is that secant method has a super linear convergence because the exponent is greater than 1 so epsilon actually grows or rather it sort of it converges as you go into the iteration of 1 step to another it does not the error does not reduce as simply epsilon i of at that stage.

But it reduces as epsilon i to the power 1.6 or 1.618 so that certainly I mean 1.618 is greater than 1 so it has faster convergence than the bisection method okay. So, we have looked at roughly 2 methods for solving these equations and it is bisection and secant they are mostly same excepting that the 2 advantage of secant method which is the guess values for the roots they do not have to subtend root you can take the guesses anywhere and then use the secant equation.

And we see that while the bisection method has a linear convergence this has a convergence which is more than more than linear that is it has an exponent which is 1.618. So, that should be more efficient in terms of its usage nevertheless even bisection method is used quite heavily and so on. But they run with the problem that if there are more roots as we just saw that we have been able to find one root.

But sometimes you know for physical problems even finding one root is enough for certain classes of problems because you just need to know that where one of the roots lie and so on. The however for both of them the convergence rate is not very good we have a third method which we are going to study which is called as a Newton Rapson method and it does not require guessing 2 roots it just requires guessing 1 root and pretty similar to the 1 that we have said in the introductory lecture on this theory of equations or solution of nonlinear equations.

And it uses just a root and the value of the tangent drawn at that point and then iterates from there and we will see that that has a better convergence and is more efficient in most of the cases. So, after that we will see some particularly physically relevant problems that are there in say for example in branches of physics and that will be the application of say Newton Rapson method.