Computational Techniques

Prof. Dr. Niket Kaisare

Department of Chemical Engineering

Indian Institute of Technology, Madras

Module No. # 04

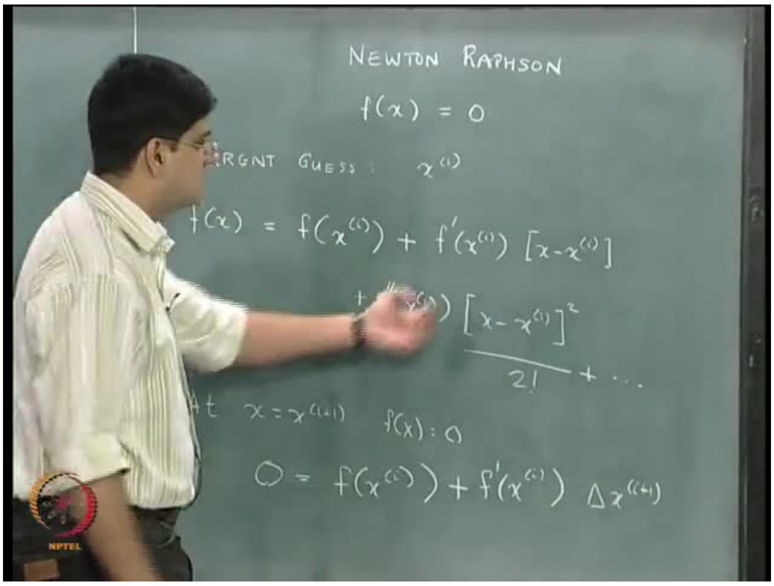
Lecture No. # 04

Nonlinear Algebraic Equations

Fixed point iteration and the bisection method: what we showed in both the fix point iteration as well as the bisection method cases, both these methods have a linear rate of convergence and then we took up the fixed point iteration method; then, when we then, when we solve that one particular expression gives us one solution, whereas the other expression leads us to the other solution; and then we check back with what we know about the sufficient condition for convergence and we observed - that - that those conditions are indeed met as sufficient conditions.

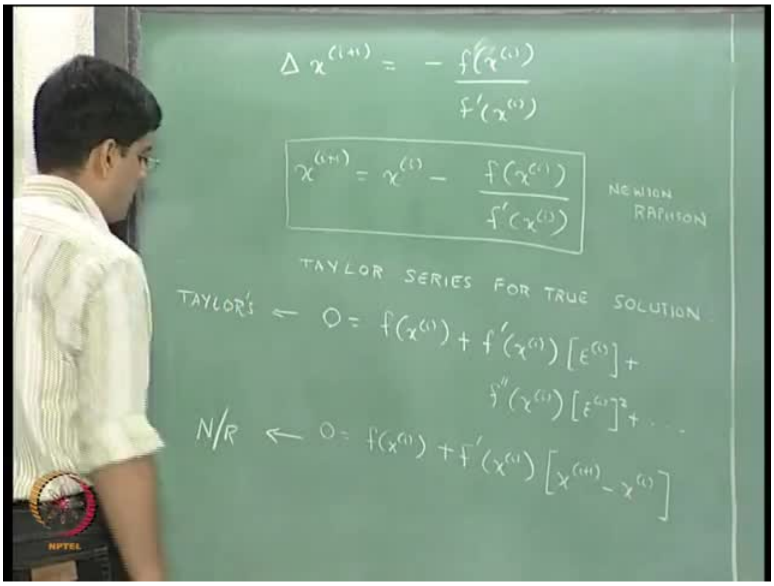
What we are going to do in this lecture is, essentially to extend that analysis to the Newton Raphson method, we will look at how fast at…, what is the rate of convergence of Newton Raphson method, how we can derive the Newton Raphson's method from Taylor's series expansion; and then we will again go back to Microsoft excel in order to demonstrate how the Newton Raphson's method works. So, let us start with Newton Raphson's.

(Refer Slide Time: 01:20)



We are interested in solving the non-linear equation f of x equal to 0, this is what we are interested in solving; let us take a Taylor series expansion of f of x around the guess current guess x i, so the current guess is x i.

(Refer Slide Time: 04:47)



So, f of x can be written as, start from this end actually, so f of x can be written as, f of x i plus f dash multiplied by x minus x i plus f double dash multiplied by x minus x i square by 2 factorial plus f triple dash x minus x i cube by 3 factorial so on and so forth; it is an infinite series, that we are going we are going to look at; so, what, this particular expression what we are going to do is, let us say that, our x i is very close to the true solution x; if it is very close to true solution x than this error x minus x i is very small; if that error is very small, we can then neglect the higher order terms compare to the first order and the 0th order term; so, what we will say is that, with - at x equal to x i or sorry - at x equal to x i plus 1, f of x equal to 0, so we will make that particular assumption in order to get x i plus 1; again f of x i is not x i plus 1 is not exactly going to be equal to 0, why it is not going exactly to be equal to 0 is because we have indeed thrown away - there is - these higher order terms.

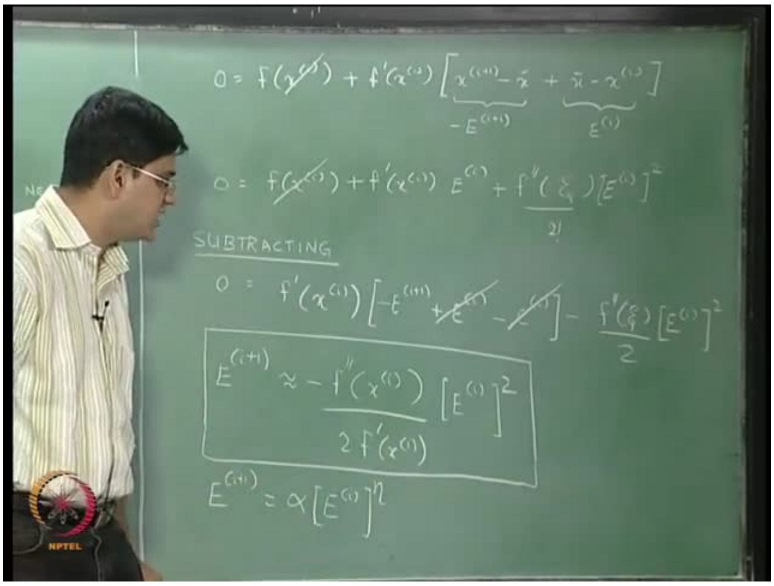
So, at x equal to x i plus 1, if f x equal to 0 means, we substitute this guy equal to 0 and this equal to x i plus 1 and then discard all the terms in that infinite series expression; when we do that, we will essentially get 0 equal to f of x i plus f dash of x i multiplied by delta x i plus 1; delta x i plus 1 is nothing but x i plus 1 minus x i; and when we rearrange that, we will get delta x i plus 1 equal to negative f of x i divided by f dash of x i, or we can write this as x i plus 1 equal to x i minus f of x i divided by f dash of x i.

So, this is essentially our Newton Raphson's method; and essentially, we have derived the Newton Raphson method keeping only the first derivative terms in the Taylor's series expansion.

So, f dash of x i essentially represents the tangent at that point; and that was the geometric interpretation that we had taken earlier; when - when in the first lecture of this particular module is when we talk out talked about a general curve and trying to use the Newton Raphson's method for this particular point on the curve, what we said was essentially what Newton Raphson's method amounts to is drawing a tangent and finding out where the tangent intersects the x axis; and again rewriting the particular Taylor series expansion; and now, for the true solution, Taylor series expansion for the true solution is f of x bar and f of x bar we know is 0, so 0 is going to be equal to f of x i plus is going to be f dash of x i multiplied by x bar minus x i which is nothing but our e i plus f double dash of x i multiplied by E i squared and so on.

So, this is going to be our expression - for the Newton - for the Taylor series expansion, for the for the true solution; remember our expression, this particular expression, who are, that we had obtained was essentially 0 equal to f of x i, that is the Newton Raphson's solution; so, what we did was, we - take this - took this particular guy on to the other side multiplied by f of x i and then took this guy again on to the other side plus f dash of x i multiplied by x i plus 1 minus x i. So, this is the Taylor series expansion; this is the Newton Raphson.

(Refer Slide Time: 08:40)



Now, what we are - going to - going to do is, essentially realize that - this guy - this particular difference can be written as the difference between the error by mean, that is the Newton Raphson's equation; we are write going to write that as 0 equal to f of x i plus f dash of x i multiplied by x i plus 1 minus x bar - minus or so - plus x bar minus x i; so, what I have done is, x i plus 1 minus x i, I have just added and subtracted x bar over there, this particular term is going to be our E i plus 1 negative, and this term is going to be equal to positive E i.

So, this is what we are going to get - in when - when we substitute; and when we subtract this particular expression from the Taylor series expansion that we obtained over here; when - when we do that particular subtraction, what we will get is, will get, I will just write a Taylor series expansion again equal to f of x i plus f dash of x i multiplied by E i plus f double dash of x i e i squared by 2 factorial plus higher order terms.

At this stage, what we will do in the Taylor series expansion is, use mean value theorem in order to replace this particular expression with f double dash of zeta, we can always find a point zeta which lies between x i and x i plus 1, such that, this particular expression is exactly satisfied without having to include any of the terms in the infinite series; so, what we have done this is an exactly correct solution, this is not an approximate solution, we have discarded, all we have not discarded all the infinite series terms, but we have chosen zeta such that, this particular expression is valid; and you can always by mean value theorem, remove, you can always find this particular value zeta, which is guaranteed to lie between x i and x i plus 1.

So, this, these are the two expressions; the first one we get from the Taylor series, sorry, first one we get by manipulating the Newton Raphson's method; the second one we have got by essentially the Taylor series expansion; we subtract these two equations and we will get these two guys are going to get cancelled and we will get f dash of x i is minus E i plus 1 plus E i minus E i minus this particular guy, is going to be 0, this gets cancelled, we take this particular expression to the left hand side and divide throughout by f dash of x i; so, what we are going to get essentially over here is, E i plus 1 is going to be approximately equal to minus f double dash of x i divided by 2 times f dash of x i multiplied by E i squared.

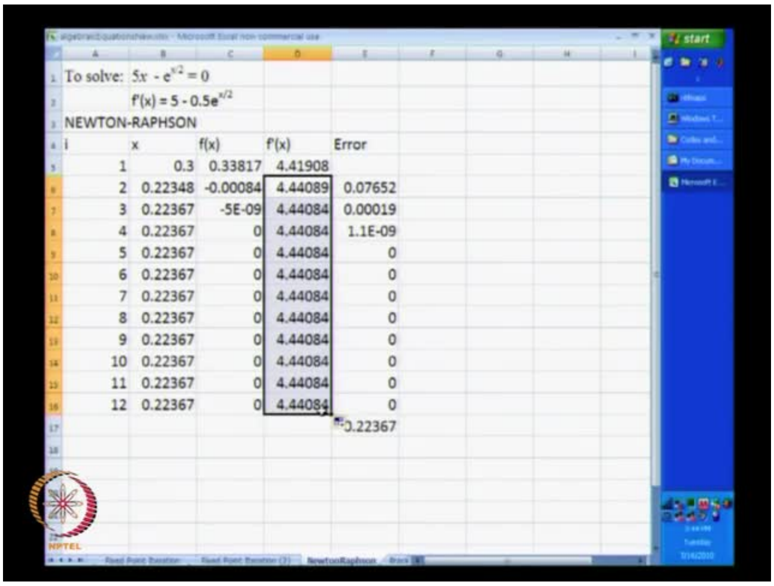
Why I have written this as an approximate sign is because we have instead of using the value zeta, we have use the value of x i under the assumption that x i and x i plus 1 do not change significantly. So, what we see is, the error at the i plus 1th iteration depends on the has a square root dependence on the error in the ith iteration; and that what - what that essentially means is that, we have a quadratic rate of dependence.

Recall what we said in the previous lecture, is what we had said is our E i plus 1 can be written as alpha multiplied by E i to the power eta; in this particular case, our eta equals 2; and therefore, what we get is essentially, what we known, what we call as the quadratic rate of convergence; and the factor that is going to determine how faster how slowly, this particular - expression - expression converges is going to be f double dash divided by 2 f dash.

So, this is the overall criterion for convergence of Newton Raphson. Now, one of the reasons for popularity of Newton Raphson is that, you will see that this the rate of convergence is much faster in Newton Raphson's compare to the rate of convergence in the fixed point iteration.

So, we will take up the numerical example in excel that we looked at - in the - in the previous lecture and we will solve try to solve it using the Newton Raphson's method.

(Refer Slide Time: 14:40)

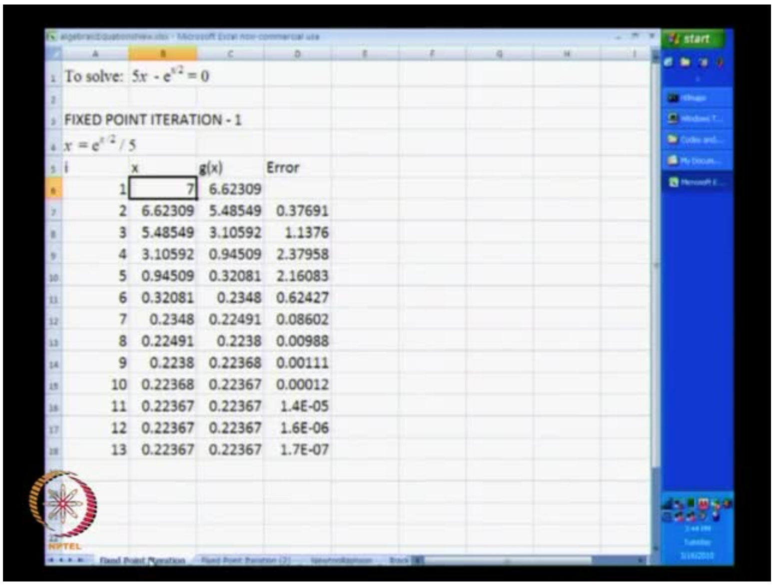


And the - same - same example that we wanted to solve in the previous lecture, 5 x minus e to the power x by 2 equal to 0 and then we take the first derivative of this and that the f dash x that we get is 5 minus e to the power x by 2 divided by 2, so 5 minus zero point five e to the power x by 0; so, the first step is the iteration number; and this is what i have been doing such the previous lecture will x 1.

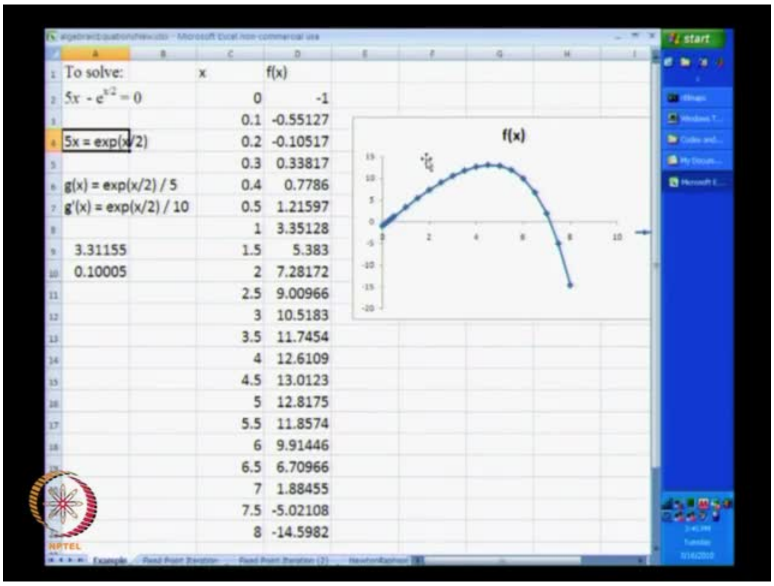
Let us start with some arbitrarily value, let us say zero point three. And our f of x is going to be equal to 5 multiplied by equal to 2 multiplied by x minus exponential of x divided by 2, that is what our f of x is going to be; our f dash of x is going to be equal to 5 minus zero point five into exp of x by - two font size to eighteen and let us right equal to - 5 minus zero point five multiplied by exp of x divided by 2.

That is going to be our f dash of x; x i plus 1 as we have written, x i plus 1 is nothing but x i minus f of i divided by f dash f i, that is what our x i was really; what that means is, equal to x of i minus f dash or f of x i divided by f dash of x i, that is our x i plus 1; again we can compute our f x, we can compute our f dash x, we have started and this error that we have is just the difference between that; and then just drag this down, also drag this particular data and we drag this guy, so what we see is essentially starting with x equal to zero point three, we are reaching our desired accuracy very quickly; the desired accuracy was 10 to the power minus 4, where very close to 10 to the power minus 4 already in the second iteration x i plus 1, x 3 is already fairly low.

(Refer Slide Time: 17:55)



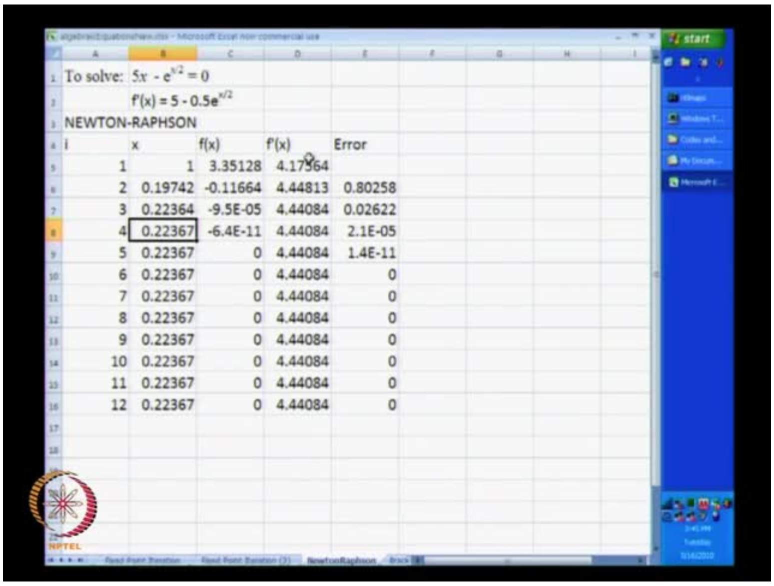
(Refer Slide Time: 18:54)



Now, if we compare it with the fixed point iteration that we did earlier; and let us do this for x equal to zero point three, this is what we did in the previous lecture; when we look at that essentially, we see that - we have - we require five iterations in order to go to the desired solution, where zero point - two two three six - two two three six eight; and in this case, it has taken much lesser number of iterations - in order iterations - in order to go to the desired solution.

Let us start with say another point, let us say which is less than the first solution; and again what we find is, we take essentially three iterations, within three iterations our solution converges our x 4 is again that is desired solution; so, what we have seen is going back essentially to this particular curve, where we plotted f of x against x; when we started on this side, we ended up with this particular solution; when we start in this side, again we are ending up - with - with that same solution.

(Refer Slide Time: 19:10)



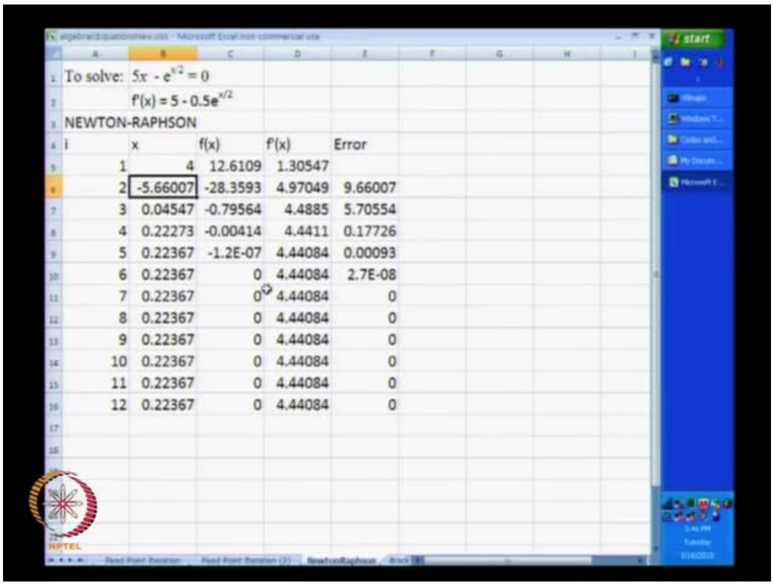
To solve: $5x - e^{x/2} = 0$

$f'(x) = 5 - 0.5e^{x/2}$

NEWTON-RAPHSON

i	x	f(x)	f'(x)	Error
1	1	3.35128	4.17564	
2	0.19742	-0.11664	4.44813	0.80258
3	0.22364	-9.5E-05	4.44084	0.02622
4	0.22367	-6.4E-11	4.44084	2.1E-05
5	0.22367	0	4.44084	1.4E-11
6	0.22367	0	4.44084	0
7	0.22367	0	4.44084	0
8	0.22367	0	4.44084	0
9	0.22367	0	4.44084	0
10	0.22367	0	4.44084	0
11	0.22367	0	4.44084	0
12	0.22367	0	4.44084	0

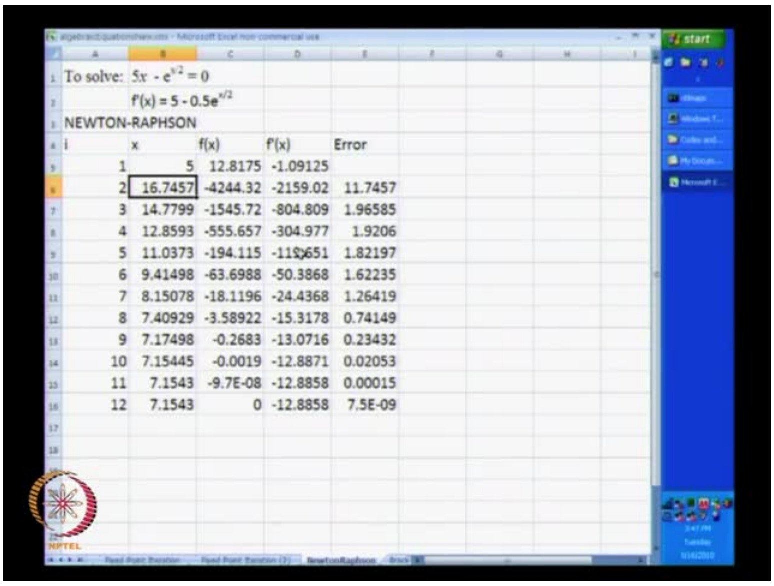
(Refer Slide Time: 20:11)



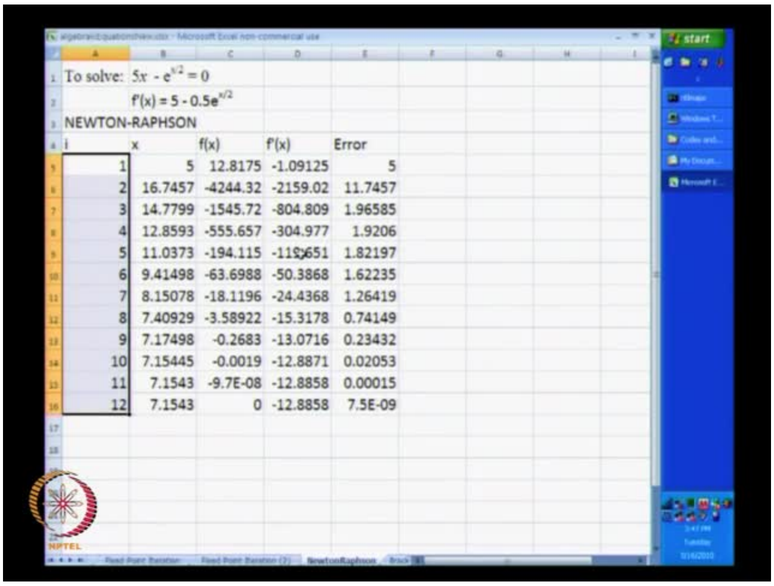
Let us increase our x 2 x equal to 1 and - what - what we see when x is increase 2 x equal to 1, still we have ended up coming at - the particular n - this solution zero point two two three's three six seven increase from x equal to one to x equal to two, again the number of iterations - that are - that are taken in this particular case - are case - is actually more than 1 more than the iterations that we are require previously, but, you will, if you still see the rate of convergence, you see that from error of two, the error has gone to zero point two that is almost of one tenth reduction beyond this; it is almost one hundredth reduction; and beyond this, it is almost one thousandth reduction or may be even more than that; so, this kind of that indicate to us quadratic rate of convergence, if or if not quadratic definitely much faster than a linear of rate of convergence; when we start let us say with the x equal to 4, again we get to the same solution zero point two two three six eight three six seven and we start with x equal to 7, this is x equal to 8, this is when we get to the other solution.

So, what we see in Newton Raphson's method is that, when we started essentially with - this this - these particular solutions, we ended up reaching this particular guy; when we started with say a solution on this side of the curve, we are reaching this particular solution.

(Refer Slide Time: 20:53)

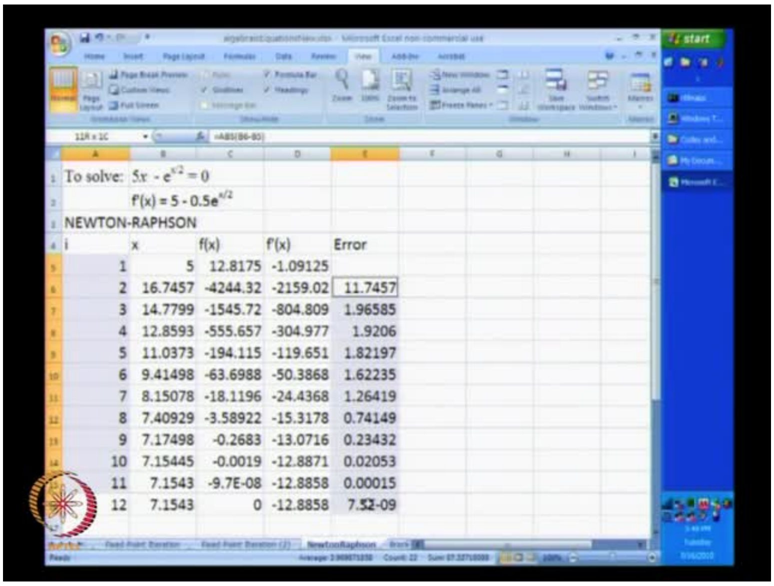


(Refer Slide Time: 21:09)

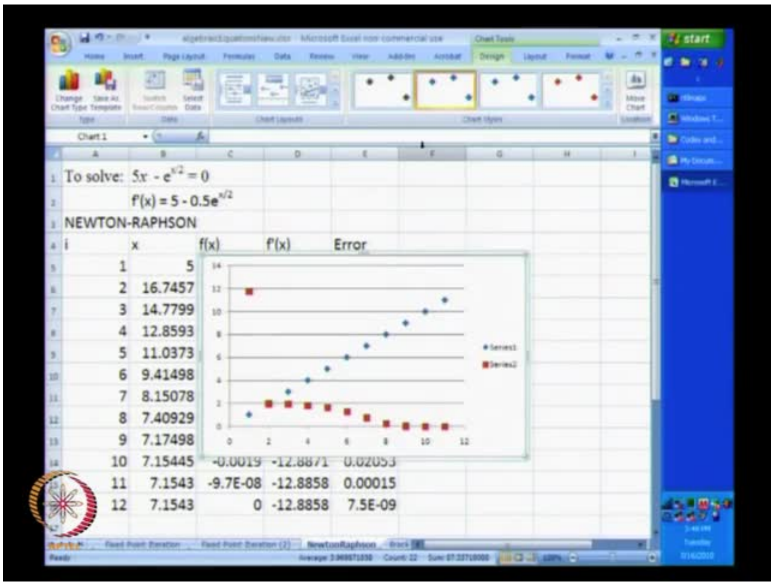


So, when we, when we start with say x equal to 6, we will again reach seven point one five four three; when we start say with x equal to 5, again we are reaching this seven point one five four three as the solution; and this is a very instructive example, where we can now go ahead and - plot - plot the error that we get over here, I have just written this this particular number so that just for the sake of completeness.

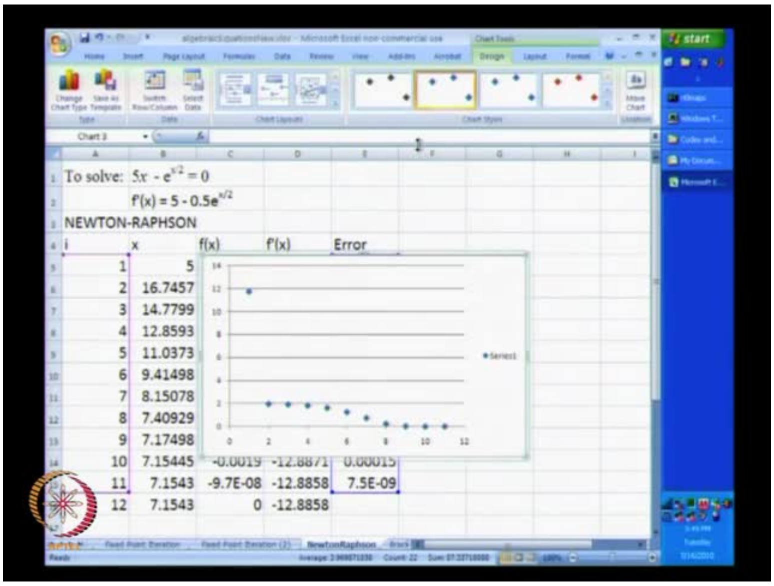
(Refer Slide Time: 21:25)



(Refer Slide Time: 21:42)

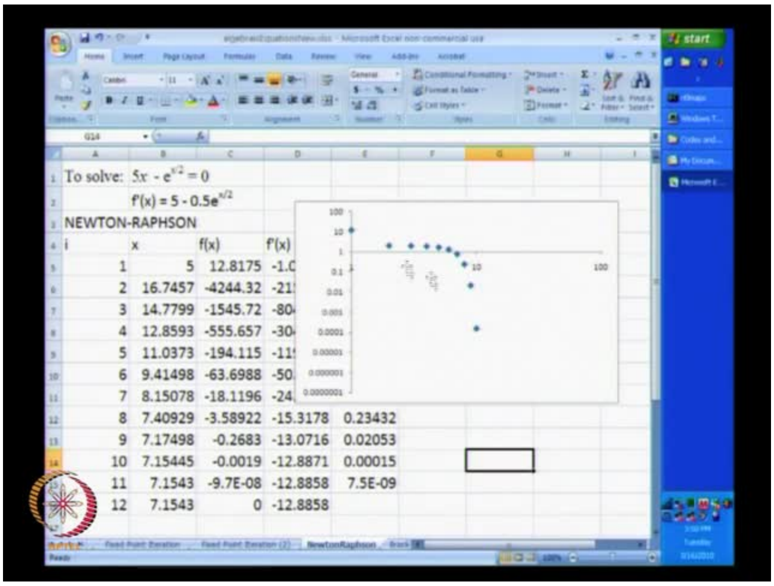


(Refer Slide Time: 22:31)

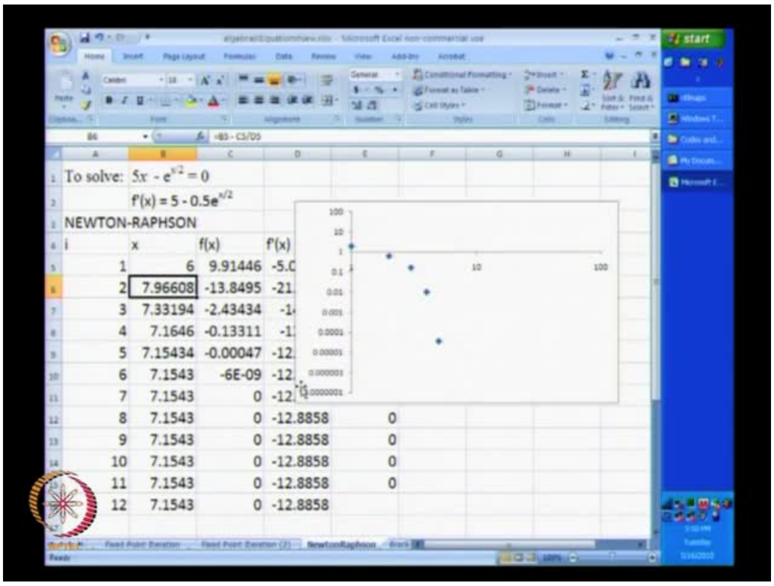


And I will just - plot - plot these guys; so, iteration number against the error - insert - insert scatter plot, let us see, will do this; these are the various errors; so, this is the plot how the errors change with iteration as we have done in the previous lecture.

(Refer Slide Time: 22:37)

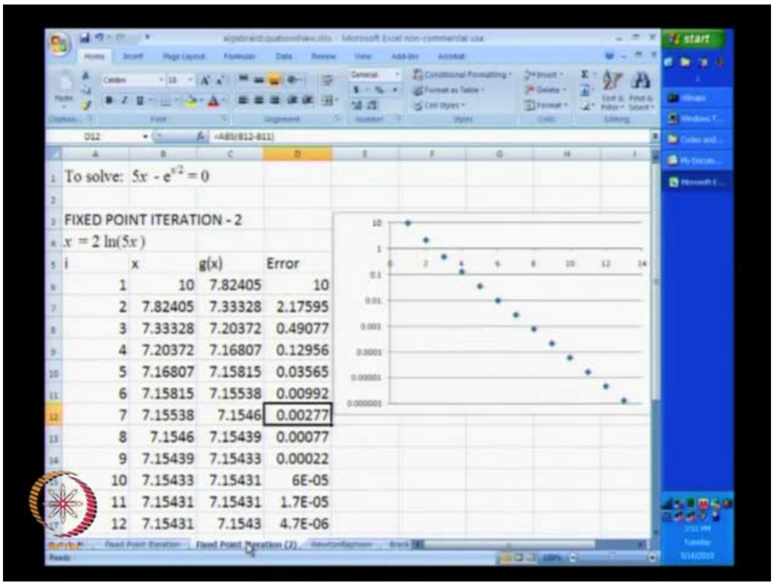


(Refer Slide Time: 22:44)

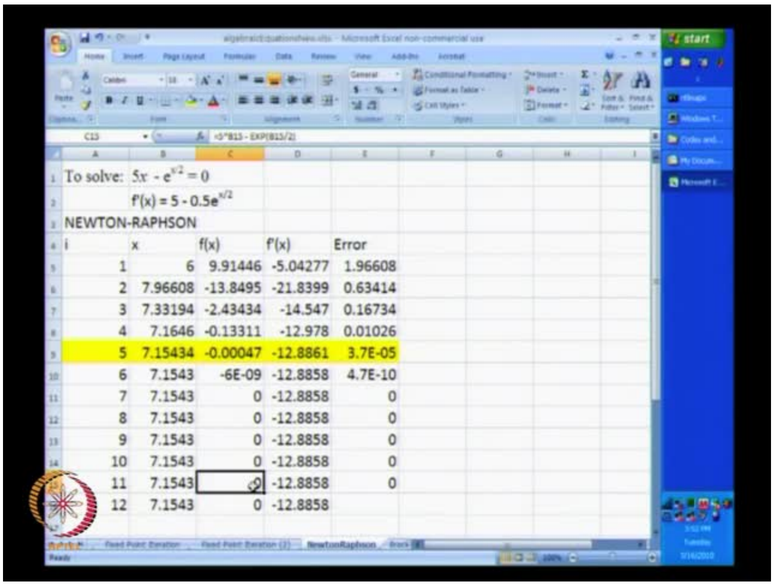


When we are doing a - log - log plot, see that what happens when we take - better - better value; so, we - do not - do not exactly want to, so this is what we get; when - when we have a particular value starting with x equal to 6, is that straight line would, have that, have an approximate slope of minus 2 in this particular case.

(Refer Slide Time: 23:18)

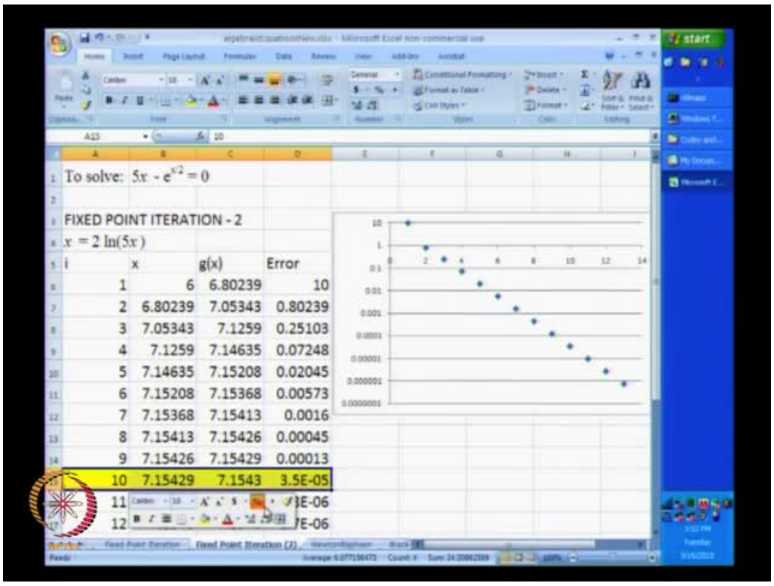


(Refer Slide Time: 23:55)

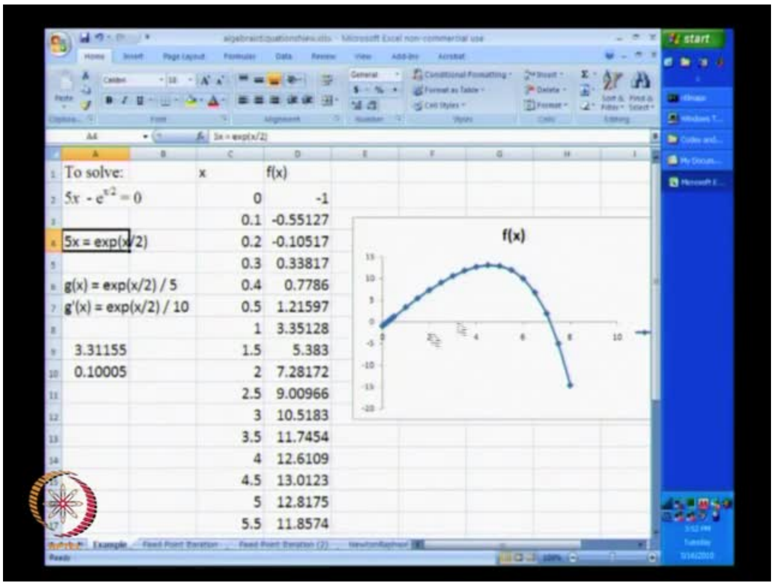


So, what that really means is that, the rate of convergence is going to be a quadratic rate of convergence in this particular example; so, none the less when we compare this, the rate of convergence of this particular method with say the fix point iteration method with the same initial conditions, so if we see the near the fix point iteration method with initial condition of 6, it requires approximately ten iterations in order to reach - the desired - the desired accuracy of ten to the power minus 4 or lesser; that happens in ten iterations, whereas in case of - Newton's - Newton Raphson's method, we require lesser number of iterations in order to - reach - reach the desired accuracy; so, we have reached the desired accuracy in five iterations in the Newton Raphson's method.

(Refer Slide Time: 24:00)



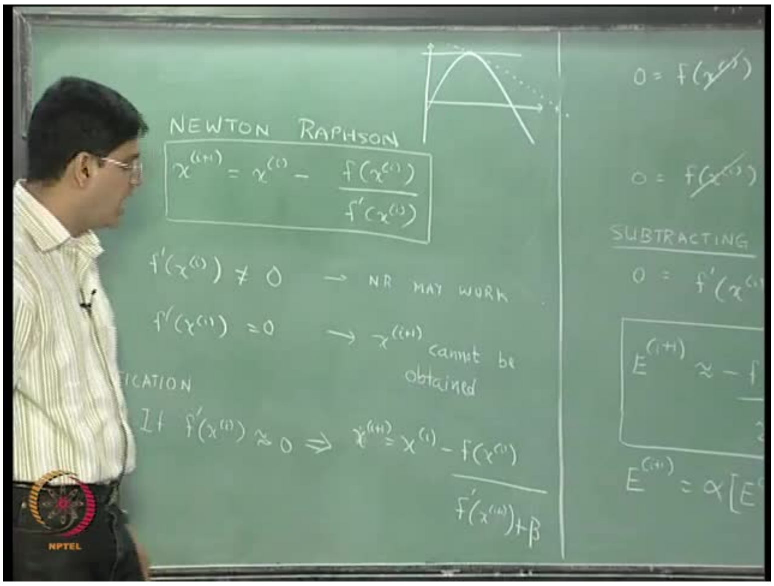
(Refer Slide Time: 24:10)



Whereas we have taken ten iterations starting with the same initial guess in case of the fixed point iteration method; another thing that we have observe in the Newton Raphson's method is, when we start off from with an x 1 value in this particular part of the graph, we will end up in on this solution; whereas when we start off in this particular part of the graph, we will end up at this particular solution; so, this is essentially what we see in the Newton Raphson's method. Now there is a problem with Newton Raphson's method and that problem arises when our initial guess is at the maxima over here.

what that means is that, the slope at this particular maxima which occurs at around zero point the maxima occurs that are around four point two two; the slope of this particular curve is 0, which basically means that, this curve is parallel to the x axis; essentially meaning that, the curve does not intersect the x axis at - at any - any point.

(Refer Slide Time: 25:12)



So, what we have is, if we go back and look at the Newton Raphson’s method expression, so when we derive this, we had assume that our f dash of x not equal to 0, that is when this particular method is going to work; however, if f dash of x is indeed equal to 0, when f dash of x i is indeed equal to 0, that is when you cannot obtain x of i plus 1; again what it physically means looking back to that particular example is, at the maxima point we have the particular line which is tangential to this curve is parallel to the x axis, so there is no point of intersection between this line and our x axis and that is where the Newton Raphson’s method is going to fail.

Now, the question is, if this is what we are going to get with Newton Raphson’s method as failing; what is it that, we can do well, what we can do is at this particular point give artificially give a small slope to the Newton Raphson’s method; so - that - there is some point at which this Newton Raphson’s method intersects.

So, the modification for…, nive modification for Newton Raphson’s method or a straight forward modification for Newton Raphson’s method is that, if f dash of x i is approximately equal to 0, then we change the Newton Raphson's method to x i plus 1 equal to x i minus f divided by f dash plus some value plus some small value beta; so, in that particular case, we will write our x i plus 1 equal to x i minus f of x i divided by f dash of x i plus beta, where beta is a small enough numbers; so, small enough number indicates essentially that we are giving it a slight slope, we are giving the tangent slight additional slope, such that, it intersects the x axis at a certain point.

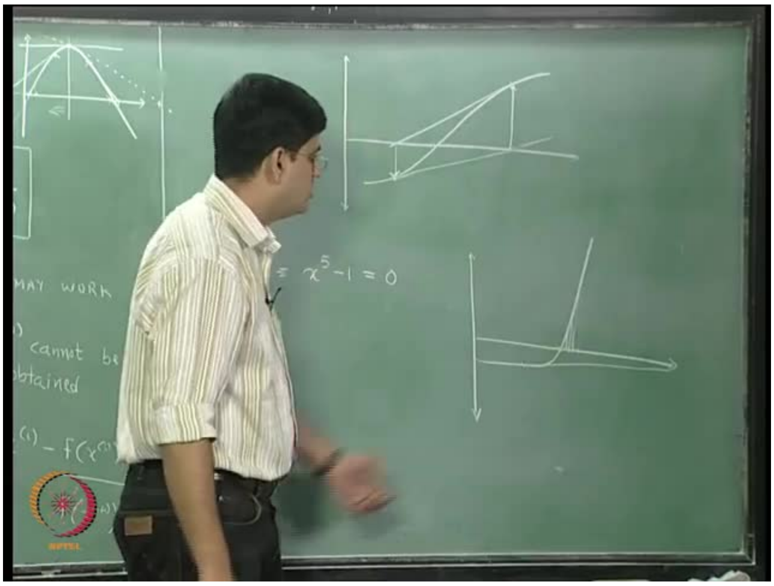
So, very popular method for minimization and for route finding called a levenberg markquadrt method or L M method uses in a more judicious sense this particular idea, not exactly this particular way of doing it as we have shown over here, but essentially the idea that the use is going to be similar.

Now, the question is, now under what conditions is the Newton Raphson's method, for the example that we looked on the excel sheet going to converge to this solution, under what condition - it going - it is going to converge to that solution.

So, basically, in a straight forward example of this type, what we will find is, when the, when - we - the initial guess is to the left hand side - of them - of the maxima at that particular point the solution is going to converge to this particular the value is going to converge to this solution; and when we are on this part of the curve, the value of the solution is going to converge to this solution; for example, with the point over here, we will draw a tangent that tangent intersects the x axis at this point, when we did not take a tangent over here, it intersects the x axis over here the tangent at this point intersects the x axis over here, and we are quickly reached this particular solution.

Likewise, if we start off with a point over here, this is going to be our second iteration, this is going to be our third iteration, and we have already reached this particular solution; so, when we start off on this part of the curve, we will essentially are going to reach this solution.

(Refer Slide Time: 30:37)



When we start off with this part of the curve, we will essentially reach that particular solution; the problem, one problem, as we had said in Newton Raphson's method is when f dash of x is indeed going to be equal to 0; there is another problem when we look at the Newton Raphson's method; so, there is another problem when we look at the Newton Raphson's method and that problem can be straighten perhaps as follows.

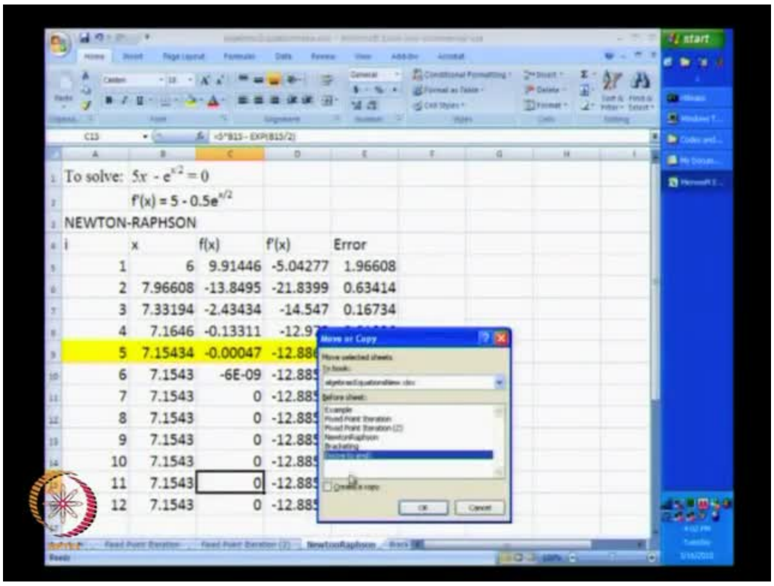
Let us say a curve is essentially, say of this type, and let us say we start off with this as our initial guess and we might get essentially a tangent - that - that looks like this; this is going to be our x i plus 1 and the tangent that we perhaps draw at x i plus 1 would end up intersecting, let us see somewhere over here; and this point again goes back to this; so, what we end up doing is, we end up getting caught in an infinitely long loop - in which - in which this particular solution throws us to this solution, this solution throws us to this solution, and keeps repeating again and again and again and we will never really reach our x bar.

Again this is a very simplified way of looking this, looking at this its often times, what happens is that, the solution may go through the three or four or five different guesses before reaching the same initial guess and it keeps repeating over and over again and we would not really get - get - a convergence.

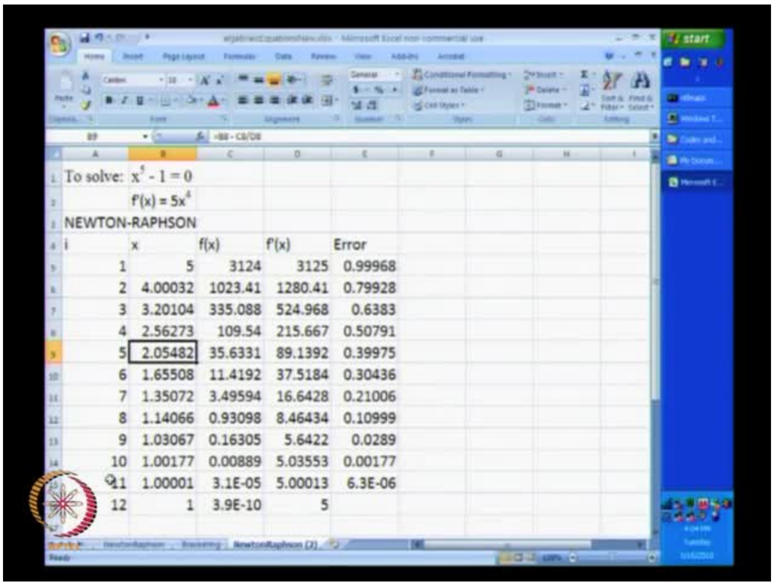
And the third set of problems is essentially going to do - have to do - with very slow rates of convergence; and an example for that is, let us say we have a curve of the form f of x equal to x to the power minus 5 minus 1 equal to 0.

Now, we know that, one of the solution for x to the power 5 minus 1 equal to 0 lies at x equal to 0 and the curve that we draw is essentially going to look somewhat like this; and this is going to be the solution x bar; and if we start at this point the will be thrown at quite a distance away, because the slope is going to be extremely small in this particular case; so, we will end up starting, let us say, at a point which is much higher over here and will end up coming at this particular location; and then beyond this point, as the iteration progresses or convergence is going to be extremely slow; and that is one possibility where our Newton Raphson's method can run into - sub - some problems; so, what will do is, we will get back to excel and we will see what that problem, where that problem occurs in the Newton Raphson's solution.

(Refer Slide Time: 33:46)



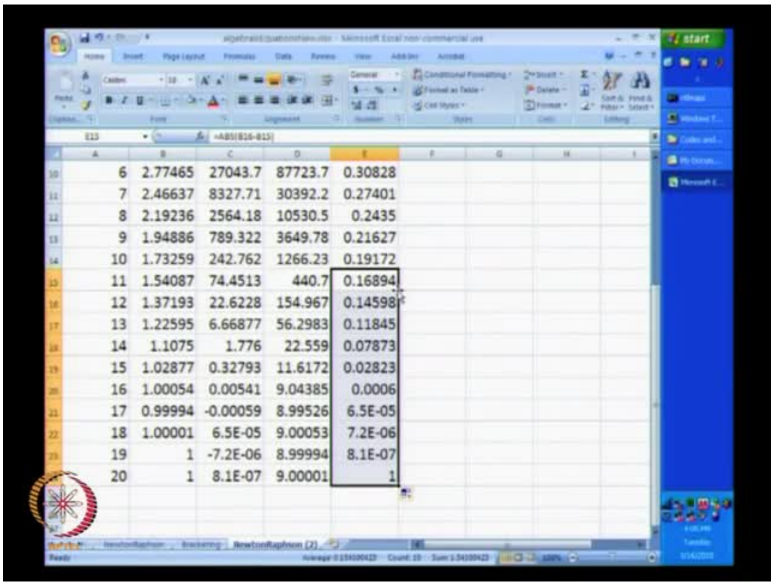
(Refer Slide Time: 33:51)



And to solve x to the power of 5 minus 1 equal to 0; so, what we are interested in solving is, x to the power 5 minus 1 equal to 0 and our f dash of x is going to be five times x to the power 4; so, this is equal to x to the power 5 minus 1; and this is going to be equal to 5 into x to the power 4.

So, let us say, we start with say x equal to zero point five, with after x equal to zero point five or next value goes at three point six, from three point six it goes to two point eight eight, two point three, one point eight so on and so forth; and it reaches the our desired solution fairly quickly in almost ten iterations; let us say, we start with x equal to 5, in this particular case, we have, we have finally ended - with - with this particular solution; compare to the previous case, we do find that in this particular case the rate of change of error is comparatively fairly slower - than - than what we had seen in the previous example and we take much longer time in order to converge.

(Refer Slide Time: 37:03)



A	B	C	D	E
6	2.77465	27043.7	87723.7	0.30828
7	2.46637	8327.71	30392.2	0.27401
8	2.19236	2564.18	10530.5	0.2435
9	1.94886	789.322	3649.78	0.21627
10	1.73259	242.762	1266.23	0.19172
11	1.54087	74.4513	440.7	0.16894
12	1.37193	22.6228	154.967	0.14598
13	1.22595	6.66877	56.2983	0.11845
14	1.1075	1.776	22.559	0.07873
15	1.02877	0.32793	11.6172	0.02823
16	1.00054	0.00541	9.04385	0.0006
17	0.99994	-0.00059	8.99526	6.5E-05
18	1.00001	6.5E-05	9.00053	7.2E-06
19	1	-7.2E-06	8.99994	8.1E-07
20	1	8.1E-07	9.00001	1

Now, if we were go to x - to the - from x to the power 5 minus 1, if we go to x to the power say 10 minus 1, in which case our f dash is going to be nine times x to the power 9; in that particular case, we are going to find that the overall convergence is going to slow down even further, so we make those changes and over here we have 9 into x to the power 9; and so, as we see over here is that, the solution is fairly slow in order in converging, let us go to, may be twenty iterations; so - when - when we started with say x equal to 5, the error started at zero point five five and as you can see that the error is decreasing fairly slowly as the number of iterations are increasing; once the Newton Raphson's method comes fairly close to the solution, let us say, of at one point zero two or something like that, then what we find is that, there is a sudden increase in the rate of convergence of this - of the Newton Raphson method.

So, initially, the Newton Raphson method is converging fairly slowly, but when it comes very close to the actual solution, at that time the convergence is going to be a rapid; we will again look at this particular example by going even further and taking initial guess as equal to 10, our initial error is one point one one as the number of iterations increase, the error as you see is coming down very slowly compare to the previous cases, the number of iterations that are required or - quite - quite a lot; and at the end of thirtieth iteration, I am quite sure we are going to converge, but we just want to look at how the convergence happens.

So, this is the error, from error of one point one one, we have decreased to an almost an error of zero point nine eight, from that we have decreased further to - small - small error values and if we go lower and lower towards the error, we find that the rate of convergence is fairly slow; Now, from this point onwards we will suddenly find that, when we come close to the actual solution - the rate of convergent really picks up now.

And that is the feature that you will see of all Newton Raphson's method, is that when we are actually very close to the actual solution, the rate of convergence becomes quadratic rate of convergence; and when we are fairly far away the rate of convergence - some - sometimes is going to be slow in the best case scenario; and in the worst case scenario, we may not have the system converge to the actual solution.

So this is what we observe in Newton Raphson's method of in a single variable. So, what we are going to do next essentially is to look at multivariable case, we will essentially cover how to extend the Newton Raphson's method and the fixed point iteration method to a general multivariable case, we will then take up an example of that multivariable case; and then we will finish off with non-linear equation solving part off our lecture of our module. Thank you.