**Numerical Methods and Simulation**
**Techniques For Scientists And Engineers**
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**Lecture 05**
**Curve fitting and interpolation of data**

So, let us look at some examples of the Newton Raphson method some of them you have seen already earlier. Now these are for you to work out I am giving you some physical problem.

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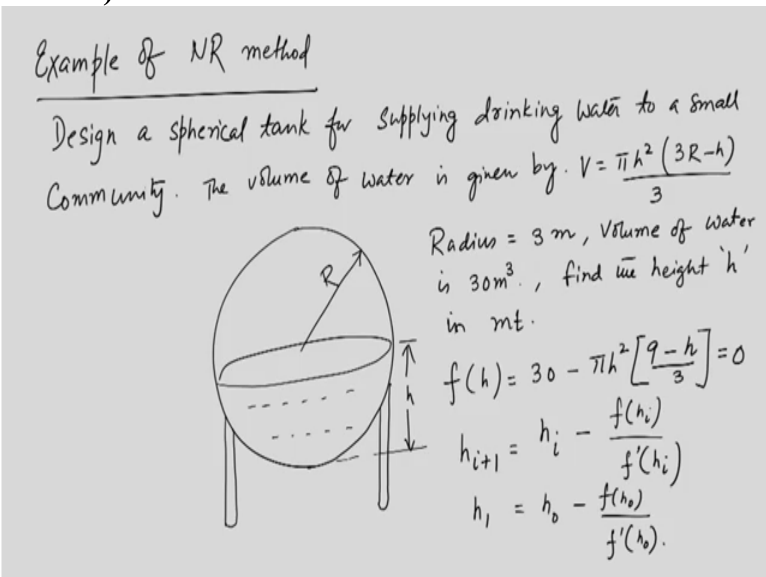


So, examples of you call it for short NR for the Newton Rapson. So, Let us say this is an engineering problem where you have to design a spherical tank for say supplying drinking water to a small village or a community, let us call it a community. And say the spherical tank has a certain you know kind of radius and it is mounted on platform and say you want to only load it up to a certain height.

Let us call that h8to be h and this radius to be R so say the volume the; volume of water is given by V equal to PI h square 3R -h divided by 3 ok, so that is a volume. And now say the radius is given so the radius is say 3 meter and the volume of water that you want is 30 meter cube that should be sufficient for a 1time serving to the community say for example and the h8of course also in meters.

So, find the h8h in meters and of course you can solve this problem but we want you to solve it by the numerical method either by the bisection or by the Newton Raphson. In particular we want for this particular case to be using the Newton Raphson method. So you want to find the h8h up till which it should be filled such that the volume is 30 meter cube and where the volume is given by this formula.

So your f of Let us call it as h which is the unknown here it is equal to 30 -PI h square which you have to find out and then you have 3R which is equal to 9 -h divided by 3 and that is equal to 0 so that is your f of h. So, what you need to know is that you need to iterate it is according to this equation h i -f of h i divided by f prime of h i, so follow that algorithm that has been told a number of times that is you have to choose a value or a guess value to begin with.

And after that, that will be your h i for a given step i or say that is the h 0 and then you get a h 1 by computing the value of the function the function is here given in front of you and the derivative of the function evaluated at h equal to h i. So, if you decide to use a value of h i which is at 0th iteration say call it h 0 then you get a h 1 which is equal to h 0 - f of h 0 divided by f prime of h 0 ok.

And then using this equation you can get h 1 from which you can get h 2 and things like that that is the thing that you should do. Just 1comment on how bad Newton Rapson can get if you unfortunately choose the initial guess value to be very sort of you know poor or rather you do not know a priori that it is a poor value but when you do not reach the desired value after a large number of iterations you understand that it is a poor value.

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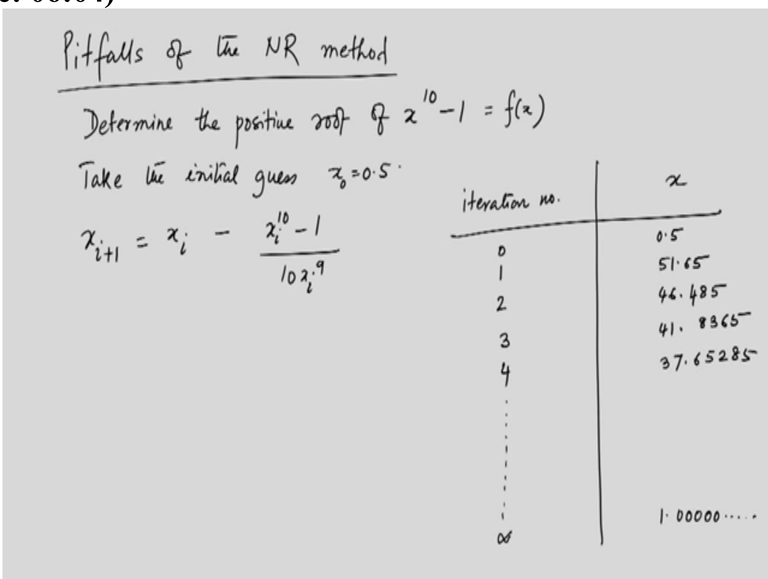


So, let me give you an example for that, so let us call it at the pitfalls of the in our method. So, say the question is determine the positive root of and this is your f of x. So, you have to find the positive root of this equation and let us take the initial guess as x equal to 0.5. So, you would iterate it according to the Newton Rapson formula which is simple which is -x i to the power 10

-1 divided by 10 x i to the power 9 and so you calculate x 1 with the help of this as x 0 let us call it as x 0.

And then we can actually form a table with iteration you can definitely check these numbers. So, it is an iteration number and versus the value of x so and at x equal to 0 of course it is 0.5 as we have decided at1, it goes into 51.65 and then for the second iteration it goes into 46.68 rather 485 and third iteration it goes into a 41.8365 and in the fourth iteration it goes into a 37.65285 and so on and only after a very large number of iteration it becomes a 1.000 which is what you require.

So, it is Newton Rapson can get particularly bad if the initial guess is a way of it would only you know sort of give you a convergent value after a very large number of iterations okay. So, we are closing now this discussion of finding roots of particularly of non-linear equations and we have seen predominantly 3 methods namely the bisection method the secant method and the Newton Raphson method.

We have discussed the convergence of each 1of these methods its seems that the Newton Raphson method out of these 3 is superior to the other 2 however you can also see the limitations of this method as we have you know illustrated in this last example and I have also given some other examples earlier. However it still is a easy enough and reliable method for calculating root only as I said earlier that if you have multiple roots then you may have difficulties.

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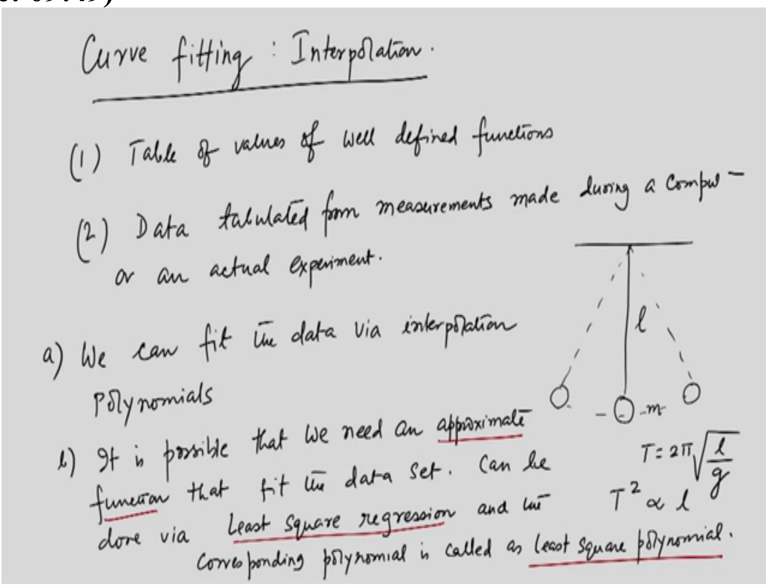


So, let us move on to another topic which is quite important it is called as the curve fitting or we are particularly interested in the interpolation a numerical interpolation okay. So, you know a table of data may actually belong to one of the following 2 following categories namely you have a table of values which corresponds to well-defined functions. So, you have a function say sine x or cosine x or a more complicated polynomial function or it could be an exponential function and you put the values of x in some discreet manner and you can generate a table of values for that particular function.

But also you can have data tabulated from measurements made during a computer or an actual experiment just to remind you of your the most basic experiment that you have probably done in the physics lab is that of measuring the value of G using a simple pendulum or what you have used it for a simple pendulum is to measure the time period of its oscillations. And what you have been instructed to is that do not give a large amplitude of oscillation to begin with because in which case the motion can become nonlinear or it can go into regime which is not really oscillatory in a simple harmonic motion.

But it could be something else so you give a small displacement which is just about at the most about 4 degrees and then you take a stopwatch and make measurements on the time period. And the time period actually has a relation with g because time period equal to t equal to 2 PI root over l by g, l is the length of the string up to the where it is hung from the ceiling. So, it is like this kind of a situation so you have a string and a bob here bob has a mass m and the string has a length l.

And you give it a displacement and then it undergoes simple harmonic motion you calculate the time period that it takes for the bob to complete 1oscillation to 1complete oscillation and that you record it in your stopwatch write it down then you know repeat your experiment and so on. And use a T equal to 2 PI root over l by g and so the mass of the bob does not appear into this particular problem it is just for you to know the value of the length where it is hung from till the point where it is attached to the bob.

And using this you can actually calculate if you plot T square versus l and you get a line the slope of that line a straight line because T Square is proportional to l you get a straight line the slope gives you 1 over g and that is why you calculate 1 over g and then invert it to get g or you are doing an experiment you are accelerating an electron in an electric field and then you are continuously changing the electric field and see that how the motion of the particle or the charged particle or the electron is getting accelerated in the in the electric field in presence of the electric field.

So, there are many of these things you routinely do or these engineering experiments that you do as a function of some parameter and these are very common in any lab and we need to we do not have and a functional relationship for the second variety that is the data tabulated from measurements. But we may want to know that how that particular data they can be fit first. Then if the data are scattered then what is the best fit of that data and can we extract a polynomial or a or a function that is known to us and predict its you know sort of value of the function at any intermediate where you have not taken the data okay.

So, all these things can be answered and so what I am trying to say is that we need a functional relationship for the for the second case where the variables are you know there is a relationship between the variables are missing. So, we actually talked about 2approaches here for fitting a curve to a given set of data points okay, all right. And in the first case the function is constructed such that it passes through all the data points that is what is wanted or that is what is desirable that you want to find a functional relationship such that your all the data points that it had passed through are being touched or connected.

This construction of a function is called as an interpolation procedure and these functions are known as the interpolation polynomials. So, we can fit the data via interpolation polynomials. And in a second case since the experimental data points are not they could be scattered they are not accurate it is it could be meaningless to talk about a single curve passing through all the points thus we can actually think about an approximate function which shows a general trend of the data set.

So, this approximate function does not need to go through all the data points it does not need to visit all the data points but it should go through that look should look like a best fit for that particular problem. So, we talked about an approximate function so let us just underline it and secondly this can be done via what is called as a least square regression and the corresponding polynomial is called as a least square polynomial.

So, let us so this is least square regression and it is a least square polynomial. So, when we have very good fit then of course we need the first one we can fit all the data using one polynomial or one particular function and if that is not possible if the experimental data or the computational data sometimes are scattered and then we need an approximate function which is done by this method called least square regression. And the polynomial that fits such an approximate or this approximate function is called as a least square polynomial you know it could just happen that we have there is no place to write here.

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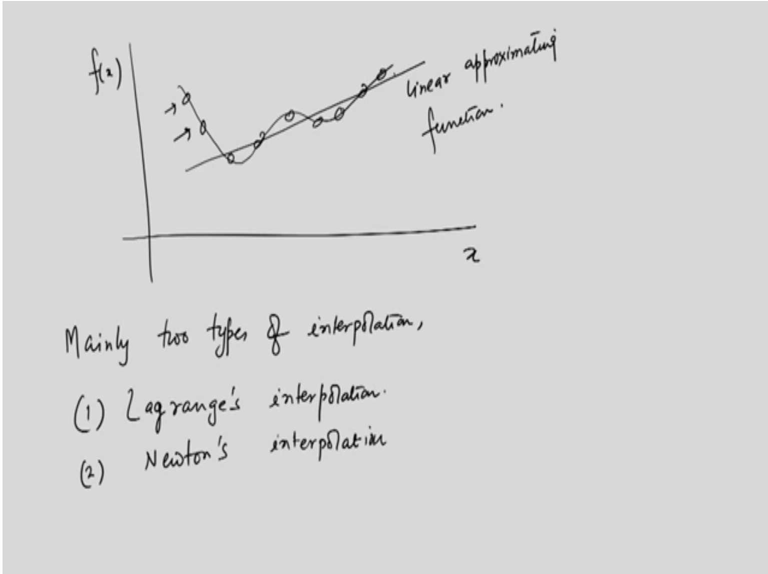


So, I will just write in the next page so these are very approximate there so you have a data like this where the data points are you know scattered like this these are the data points and then you actually can talk about a function which goes through most of the data points or through captures most of these data points excepting may be these 2 but otherwise they are very close to this data points.

So, there is a linear approximation function approximating function. So, this is your f of x versus x all right. so we are going to talk about mainly 2 types of interpolation namely Lagrange's interpolation and number 2 say Newton's interpolation okay. So, these are the 2 methods that we are going to discuss. Let us first look at the linear interpolation which will make things easier for you to understand what's going to come up later.

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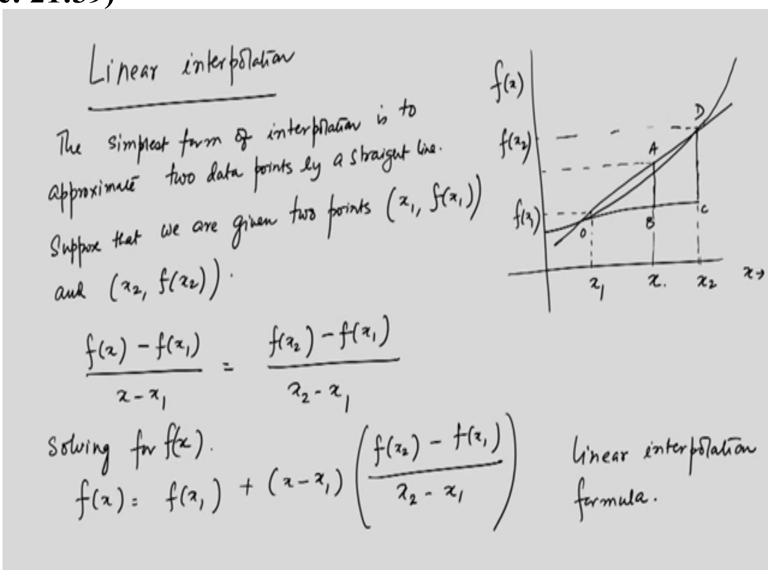


So, we are talking about a linear interpolation and consider this plot. So, there is a function like this and you want to express it as a as a linear function so this is x 1 this is x 2 to not mind this slight curvature of the straight line that I wanted to draw maybe I will try to draw a better one that shifts my x 2 but does not matter okay. So, that is fine and that is your f x versus x and we can of course do a linear interpolation of data by 2 data points this is of course a minimum that we need are we showing 2 data points.

Just to approximate 2 data points by a straight line. Suppose that we are given 2 points x 1 fx 1 of course these are fx 1 and this is f x 2 x 2 fx 2 we have linearly connected these 2points as you see there. So, basically now let us take an intermediate point here and call that as x okay. So, we can use the similar properties of triangles here and of course and the one that is here so we are talking about the 2 triangles say O A B and C D okay.

So, it is OAB and OCD the similarity of this triangles one can write down fx -fx 1 by x -x 1 it is equal to f x 2 -f x 1 by x 2 –x 1 and solve for x or rather f of x, so f of x become f of x 1 +x –x 1 f of x 2 -f of x 1 divided by x 2 –x 1 this is the best you can do using 2 points. So, you can linearly interpolate between these 2 points and you would get a function which is given by f of x equal to f of x 1 the value of the function at the x 1 point x –x 1 and all these f x 2 -f x 1 divided by x 2 –x 1 ok. So, this is called as a linear interpolation formula okay.

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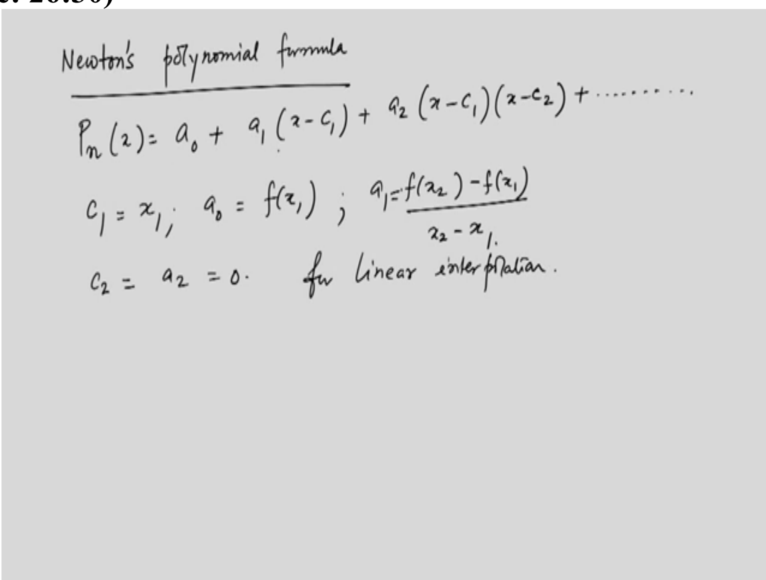


So let us see and it is called as a Newton's interpolation formula so Let us write down this as Newton's polynomial formula so we have just simply written down the linear formula but the polynomial formula when you have a more complicated function can be written as so, you have a P n x so it n stands for basically any thought a polynomial a 0 +a 1 x - some C 1 +a 2 x -C 2 x -C 1 x - C 2 and so on okay.

So, what is what are these so your C 1 is equal to x 1 a 0 is nothing but value of the function at x 1 a 1 is nothing but the slope which is f x 2 -f x 1 x 2 –x 1 and of course your C 2 equal to a 2 equal to 0 for linear interpolation. So, we stopped the function at this uptil this and we take the linear and if you want to go beyond linear then you have a quadratic and a cubic and aquatic and so on terms.

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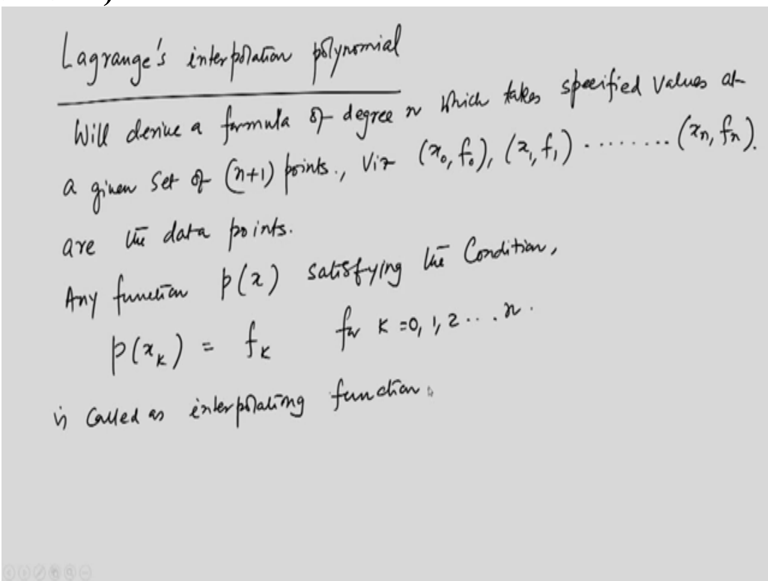


So, let us look at the Lagrange's interpolation polynomial that is the first method that we do so we will derive a formula of degree n which takes specified values at given set of n +1 points this what I was telling you earlier that you have performed an experiment and have got a set of data points and data points or n +1 data points and we want to fit it by a polynomial. Right now we are describing a method called as a Lagrange's interpolation polynomial.

And this polynomial will write down but then polynomial will have to take specific values at the data points that you have found out from an experiment ok. So, this polynomial has to obey or has to have that value at the given data points which are experimental quantities. So, for example you have x 0 f 0 you have a x 1 f 1 and continuing all the way you have a x n f n so these are the data points okay.

And so any function P x satisfying the condition P of x k equal to f k for k equal to 0 1 to n okay is is called as the interpolating function this is what we said.

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Let us consider a second order polynomial,

$$p_2(x) = b_1(x-x_0)(x-x_1) + b_2(x-x_1)(x-x_2) + b_3(x-x_2)(x-x_0).$$

We are given $\underbrace{x_0, x_1, x_2}$ and $\underbrace{p_2(x_0), p_2(x_1) \text{ and } p_2(x_2)}$.
$f_0 \quad f_1 \quad f_2$

$$p_2(x_0) = f_0 = b_2(x_0-x_1)(x_0-x_2).$$

$$p_2(x_1) = f_1 = b_3(x_1-x_2)(x_1-x_0).$$

$$p_2(x_2) = f_2 = b_1(x_2-x_0)(x_2-x_1).$$

$$p_2(x) = f_0 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)} + f_1 \frac{(x-x_2)(x-x_0)}{(x_1-x_2)(x_1-x_0)} + f_2 \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}$$

$$= f_0 l_0(x) + f_1 l_1(x) + f_2 l_2(x) = \sum_{i=0,1,2} f_i l_i(x)$$

To make things you know more concrete and easily understandable let us take a second-order polynomial, P 2 x its equal to say b 1 will tell you what these are these are coefficients x -x 0 x -x 1 +b 2 x -x 1 x -x 2 and a b 3 and x -x 3 and x -x 2 x 0 okay. So, what we are given we are given 3 points x 0 x 1 and x and this is I wrote something wrong here this cannot be 3 we are just given 3 points x 0 x 1 and x 2 so this has to be x -x 2 these 3 points we are given and the value of the function at these 3 points.

And P 2 that is the second order 2 stands for order as I said and x 0 and P 2 at x 1 and P 2 at x 2 so these set of points and their corresponding values are there are available to you. So, these are the points  let us call the P 2 x 0 to be f 0 and if I put x equal to x 0 the first term vanishes and the third term vanishes so both these terms vanish and we get x 0 -x 1 and x 0 - x what is it so we have x 0 -x 1 and x 0 -x 2, so that is the second term only survives.

Now P 2 at x 1 let us call it as f 1 so we will call it as f 0 f 1 and f 2. So, f 1 will put now x equal to x 1 again the first term and the second term vanish leaving aside the third term so this will be b 3 x 1 -x 2 and x 1 -x 0 so that is your f 1 these are all like known values because all these x 0 x 1 x 2 is unknown. Similarly a P 2 x 2 which we call as f 2 now we will put x 0 x 2 x equal to x 2 this the last 2vanish giving me x 2 -x 0 and x 2 -x 1 so these are the 3 values we get.

Now we you see there are 3 unknowns so which are b 1 b 2 and b 3 so we can solve for b 1 b 2 and b 3 and substitute into this equation for the polynomial so my P 2 becomes equal to f 0 x -x 1 x -x 2 divided by x 0 -x 1 +f 1 x -x 2 x -x 0 x 1 -x 2 x 1 -x 0 +f 2 x -x 0 x -x 1 divided by x 1 x 2 - so we have x 2 -x 0 and x 2 -x 1 ok. So, I have f 0 and this function f 1 and this function and f 2 and this function ok.

So, we are so Let us just show you using laser pointer maybe so we have a function here and we have of interpolating function here and we have an interpolating function here these are called as a Lagrange is interpolating factors. Let us see, so this can be written as f 0 l 0 x +f 1 l 1 x +f 2 l 2 x and so on. If you like this is like a sum over i equal to 0 1 2 f i l i x and if you go to larger polynomial that is more than second order you would have more terms here in a second order typically we have 3 terms.

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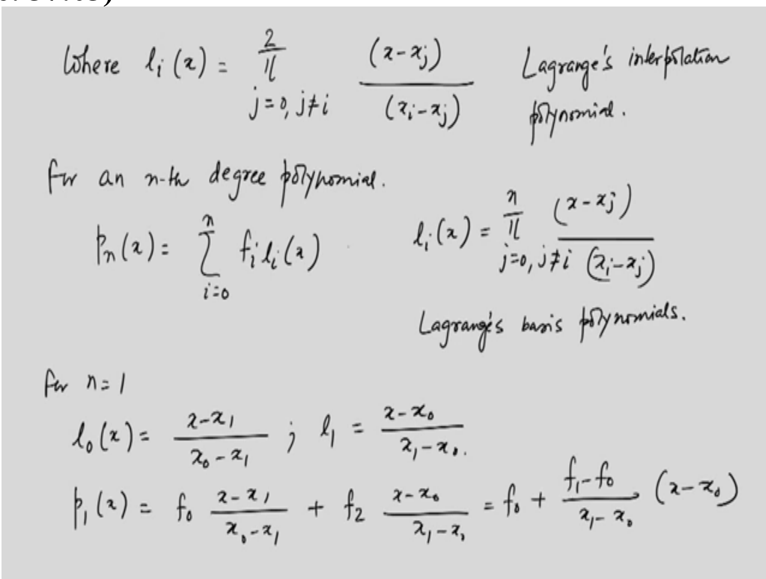


So, a general formula for this l i which we have written as l i x its equal to product over j equal to 0 from j equal to 0 and j not equal to i up to j equal to whatever I mean here it is 2 so I am writing 2 it is x –x j and x i –x j you remember that j is not equal to i because the denominator then blows up so for an nth degree polynomial P n x is nothing but equal to this is like i equal to 0 to n and f i l i x this is and these allies are called as a Lagrange as as I told earlier Lagrange's interpolation polynomial.

And in this particular case where for a general an eighth order polynomial we have it like this j equal to 0 to n with j not equal to i we have a x -xj and we have a x i –x j the form remains the same excepting that now the product is over a larger number of terms and these are called as the basis Lagrange basis polynomials all right. So, things are quite simple so let us just check for n equal to 1 n equal to 1 of course we will have if we are talking about a linear polynomial then we'll have of course have 0 and 1 the 2 values.

So, l 0 will l 0 of x, x -x 1 x 0 -x 1 and l 1 is equal to x -x 0 x 1 -x 0 so using l 0 and l 1 a linear polynomial can be written as x –x 1 x 0 –x 1 which you have been exposed to earlier is x –x 0 x1 –x 0 if you simplify it, it becomes f 0 +f 1 –f 0 divided by x 1 –x 0 into x –x 0 see that is the formula that we have given here the same formula that appears here in the last line. So, that is for the linear n equal to 1 you go to quadratic you will have one more term and things like that and of course you will get a quadratic function in x or you get a cubic function or you get aquatic function depending on the order of the polynomial that you want to consider for a given set of data points.

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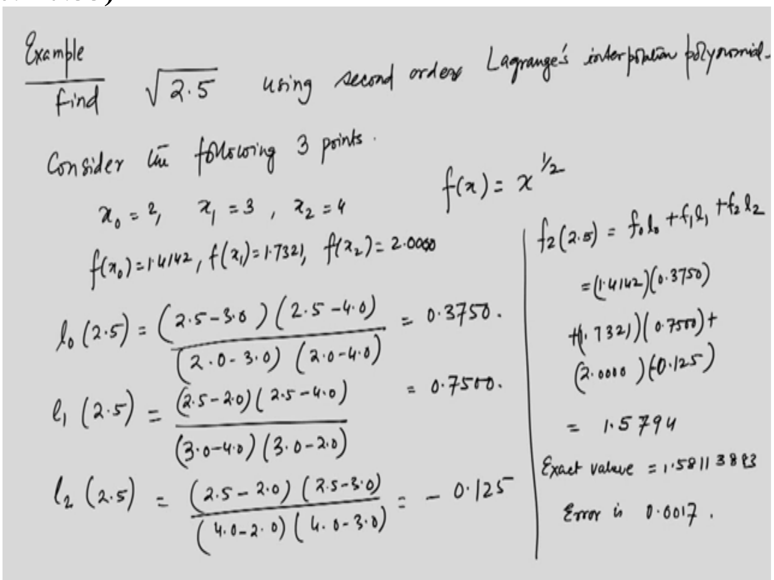


Let us just look at a interesting problem when we were young in school I do not remember that we have been taught how to calculate the square root of decimal numbers and this I do not remember maybe that was there in books but now of course children know how to calculate there are algorithms and there are various techniques that are given. So, Let us calculate the square root of 2.5 find using a second-order polynomial Lagrange's.

So we have to because we are talking about a quadratic fit we need 3 numbers or 3 quantities so let us talk about 3 consider the following 3 points namely x 0 equal to 2, x 1 equal to 3 and x 2 equal to 4 so we have taken 2 to be on the you know the larger side of 2.5 and 1 to be lower than 2.5 but it does not matter you can take it as you wish. So, this is equal to important thing is that your 2.5 has to be subtended somewhere between these 3 values.

So, you have a function like this so if you calculate from what we have prescribed for l 0, l 1 and l 2 in this thing because we are talking about the second order so you should take these formula that appears in the p 2 expression and one calculates l 0 at 2.5 rather; so let us just first write down along with this before we write this, so let us write down f of x 0 equal to 1.4142 f 1 x1 equal to 1.7321 f of x 2 equal to 2.0000 could have simply written 2 but since we are doing numerical methods we should be consistent in defining the decimal places for each one of these.

We have kept 4 decimal places here and so l 0 the Lagrange's basis so to say at evaluated at 2.5 is 2.5-3.0 2.5-4.0 see the formula once that we have done so x -x1 x is points 5 x 1 is 3 so it is

2.5 -3 2 .5 - 4 and so on that is what is written there and 2.0 -3.0 and we have a 2.0 - 4 .0 and this becomes .3750 l 1 for example is you can again write it I am skipping it for now and so it is .7500 so let us just write it for completeness 2.5 - 2.0 and a 2.5-4.0 and then a 3.0 - 4.0 and 3.0 - 2.0 and this will give you a .75and then l 2 which is 2.5 is equal to 2.5-2.0 and a 2.5-3.0 you do all yourself in order to be convinced very simple thing 2.0 and 4.0 - 3.0 so that becomes -0.125.

So, that gives us the f 2 at 2.5 is equal to f 0 l 0 + f 1 l 1 + f 2 l 2 and that gives me 1.4142 into . 3750 and + 1.7321 multiplied by a .7500 + 2.000 multiplied by 10.125 okay. So, if you simplify that that becomes equal to 1.5794 whereas the exact value is equal to 1.58113883. So, if you look at the error so error is about .0017 and so it is using just a second-order polynomial you get results that are very close.

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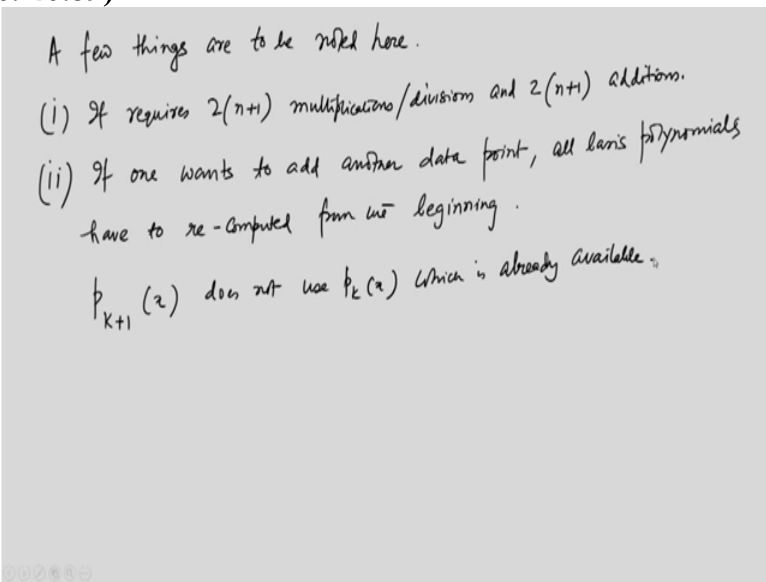


Few things are to be noted here it requires 2 into n +1 so that is 2 n +2 multiplications / divisions and equal number of addition or subtractions I mean basically additions, additions of numbers I mean subtraction if there is a sort of minus sign that comes and you have to take care of it so that is an impediment that there are so many calculations or so many computations have to be done by the computer and division as we know is always hassle some procedure especially when you want to get you want to divide by small numbers.

The more you know stringent condition that it has is that if you want to add 1more data point then you have to recompute everything once again because these Lagrange's basis polynomials will not allow you to have one more data point into the into your calculation. So, if one wants to add another data point all basis polynomials have to be recomputed from the beginning. So, basically what it is trying to say is that if you have a P k +1 that does not use P kx which is already available okay.

So, we will go ahead with this and show some more examples and also use the inter neurons interpolation formula for this particular purpose you.