**Numerical Ananlysis**
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**Lecture 10, Part 2**
**Numerical differentiation 2**
**Method of Undetermined Coefficients**

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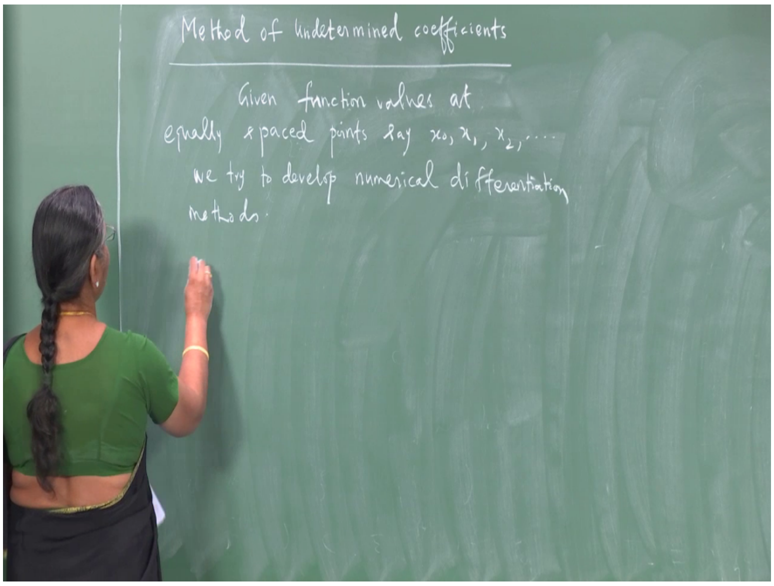


Given function values at equally spaced points say x 0, x 1 etc. So we try to develop numerical differentiation methods. How are we going to do this We write out the method that approximates say derivative of the function f Say the first derivative involving function values at some points and require that the unknown constants which appear in this method are determined in such a way that the resulting numerical differentiation method is exact for polynomials upto certain degree. This is how we determined the coefficients which are unknown.

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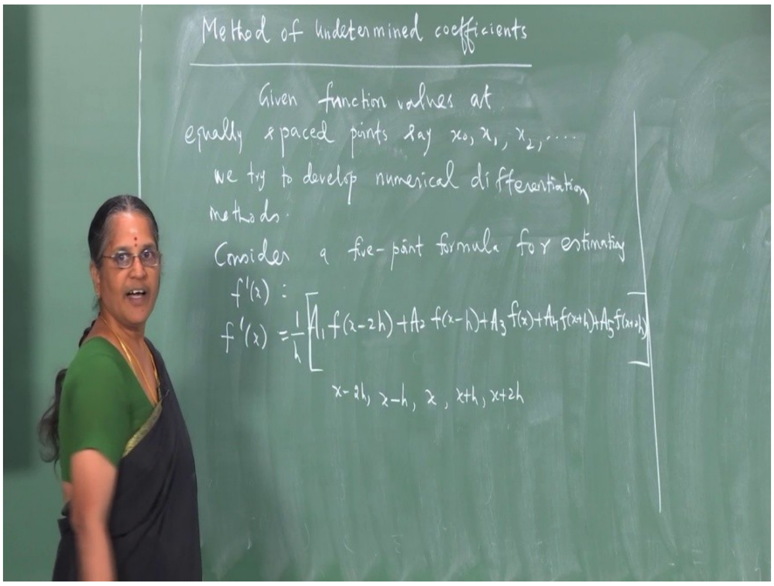


So let us consider the following five points formula. Suppose say I am interested in considering a five point formula for f dash (x) for estimating f dash (x). Let us take the formula as I want f dash (x) to be estimated in such a way that it is A 1 times f(x minus 2 h)plus A 2 into f(x minus h) plus A 3 f(x) plus A 4 f(x plus h) plus A 5 into f(x plus 2h) say divided by h. Say I want to construct a formula for f dash (x) in this form so what are the points that are involved x minus 2h x minus h x plus h x plus 2h and information about the function values are available to me at a set of these points.

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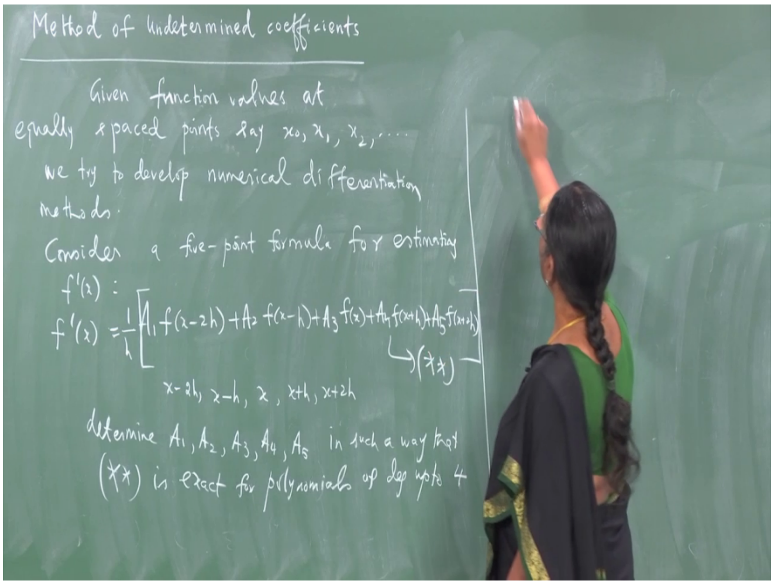

So I take a linear combination of these values function values and what is my requirement now I determine this constants A 1, A 2, A 3, A 4, A 5 in such a way that this method which I call as double star is exact for polynomials of degree upto let us see how many constants do we have there are 5 unknown constants to be determined. So we require 5 conditions to determine these 5 constants.

So we require we enforce the condition at a method double star is exact for polynomials of degree upto say 4. So we have a constant polynomial the first degree the second degree the third degree and the fourth degree polynomials So they will give us 5 conditions to determine these 5 constants.

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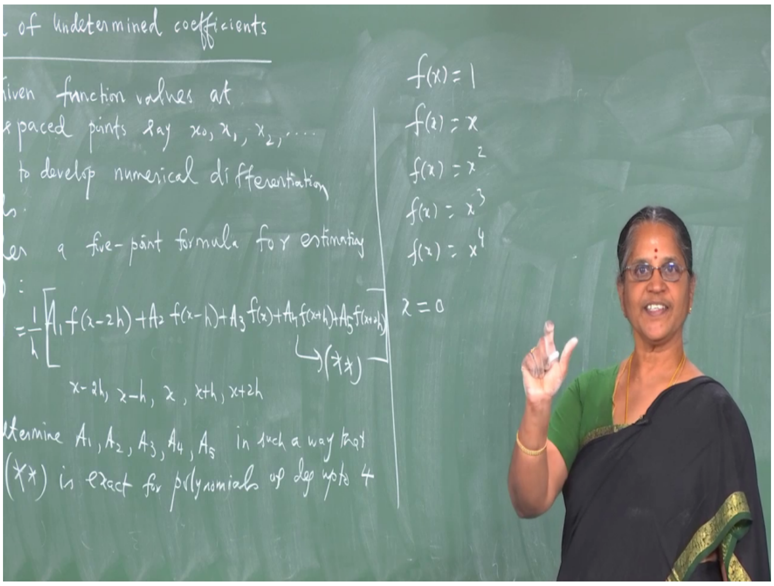


It is enough to ensure that the method double star is exact for Polynomials given by f(x) is equal to 1 x x square x cube and x to the power of 4.Because the expression involves only function values and they appear linearly and secondly we would like to obtain this method in such a way that it should be independent of any any shift of origin.

And so we consider this method with x is equal to zero and derive this method and thirdly the method that we are going to obtain should be independent of the step size of h. And therefore we take h is equal to 1 in this method and then obtain the numerical differentiation method for approximating f Prime of x.

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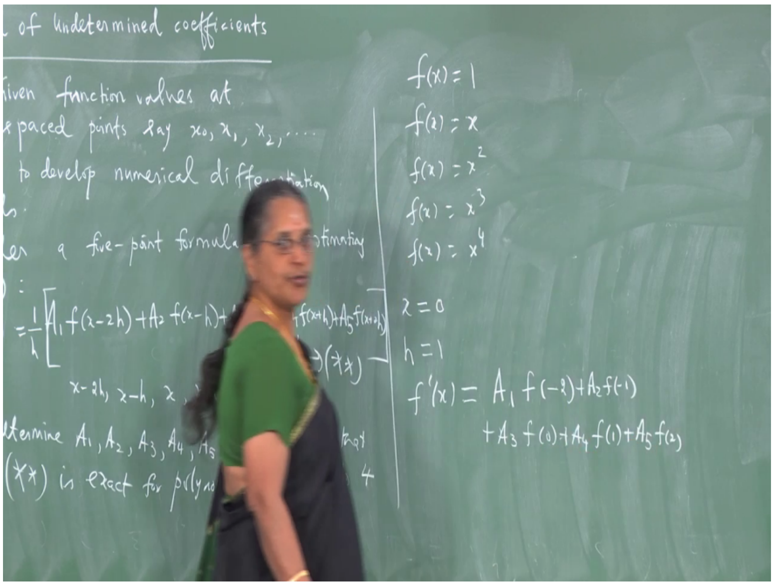


So we take as prime of x must be of the form A1 into f prime (x) is equal to A 1 f h is 1 and x is 0 so f at minus 2 plus A 2 f of ( minus 1) plus A 3 f (0)plus A 4 into f(1) plus A 5 into f at 2.

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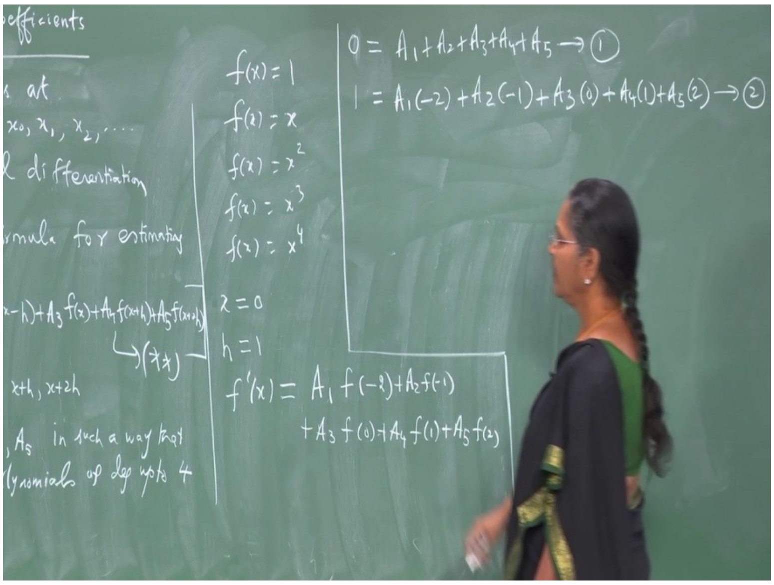


So let us substitute f (x) given by these and arrive at the conditions where f(x) is 1 and then this gives u f prime x is 0. And therefore it give you A 1 plus A 2 plus A 3 plus A 4 plus A 5 So that gives you the first equation.

When f(x) is x f prime x is 1 and that will give you A 1, A 2 f(x) is x so f(minus 2) will be minus 2 plus A 2 into f(minus 1) plus A 3 f(0) plus A 4into f (1) plus A 5 into f (2) so that gives you the second equation.

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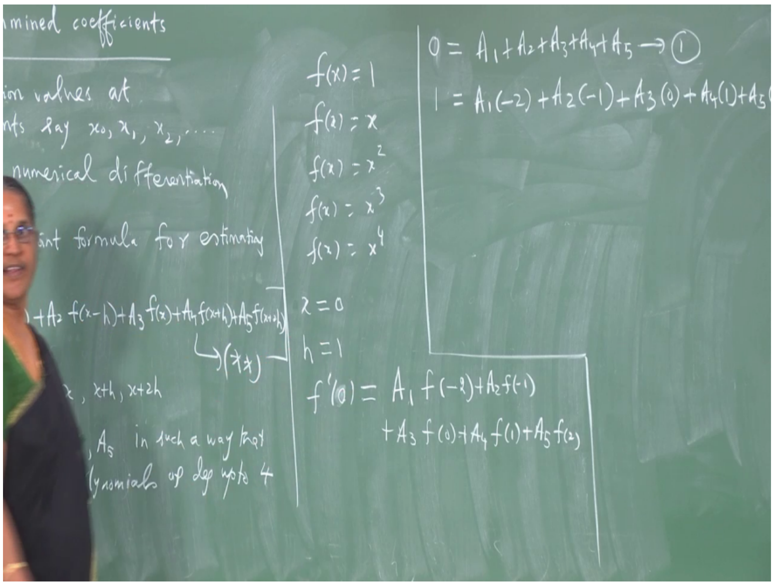


When f (x) is x square so f prime x is what. We have take x to be 0 so f prime evaluated at 0 is given by the right hand side.

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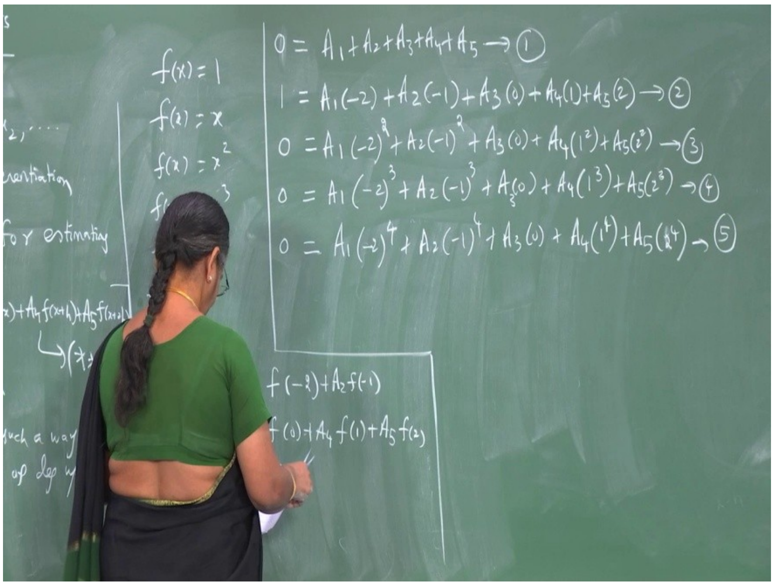

So when f (x) is x square f prime is 2x evaluated at 0And that is equal to A 1 into x square. So f (minus2) is (minus 2) the whole square plus A 2 (minus 1) the whole square plus A 3 into 0 plus A 4 into 1 square plus A 5 into 2 square.

Then when f(x) is  x cube it is 3x square so at 0 will give me 0 equal to A 1 into it is x cube so (minus 2) the whole cube ( minus 1) the whole cube plus A 3 into 0 plus A 4 into (1) cube plus A 5 into( 2) cube. And finally when f(x) is x to the power of 4 4(x) cube is its derivative.

So at 0 it will be 0 so that will give you (minus 1) I mean A 1 into (minus 2) power 4 plus A 2(minus 1) power 4 plus A 3 into 0 plus A 4 into 1 power 4 plus  A 5 into 2 to the power of 4 that gives you fifth equation So we have five equations to solve for A 1 A 2 A 3 A 4  and A 5.

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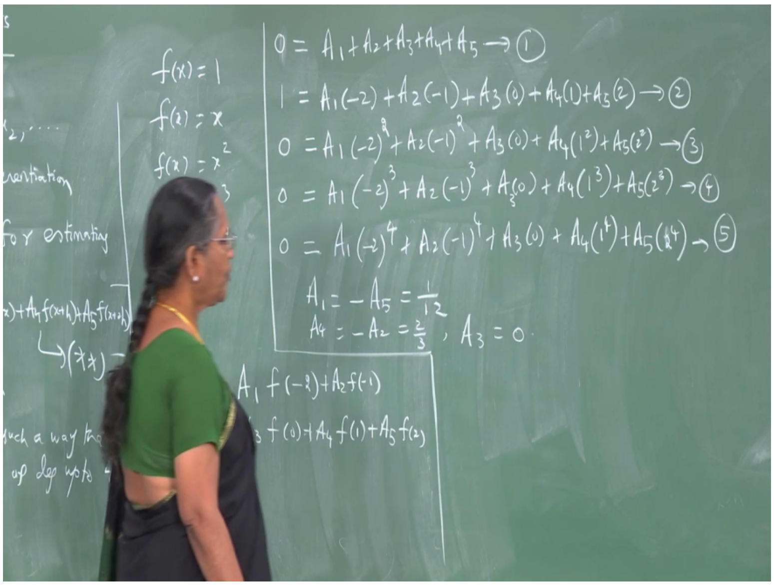


So when you solve these equations you end up with the solution as A 1 is equal to the minus A 5 equal to 1 by 12 and A 4 is minus A 2 and that turns out to be 2 by 3 and A 3 is 0.

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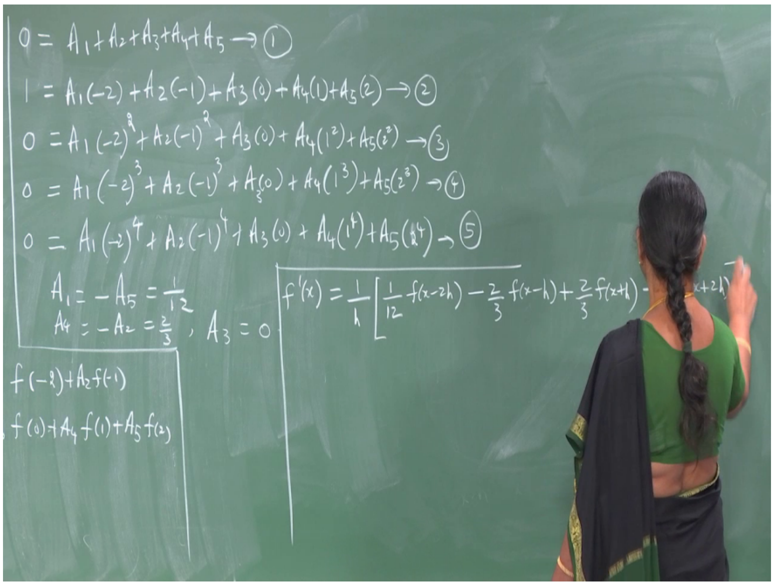


So this tells you that you have a differentiation formula for f prime (x) such that it is 1 by h into [ A 1  A 1 is 1 by 12 into f(x minus 2h) plus A 2 that is minus 2 by 3 into f at( x minus h) plus A 3 that is 0 plus A 4 which is 2  by 3 into f( x plus h) then plus A 5 (minus 1 by 12) into f at( x plus 2h)].

So it is important to see the class of function for which this method is valid that is one thing and also to see the order of accuracy of this method which essentially means that we have to obtain the error term in this approximation. So let us work out the details of error that is incurred in approximating the first derivative f prime (x) in terms of the values of the function with involving 5 points.

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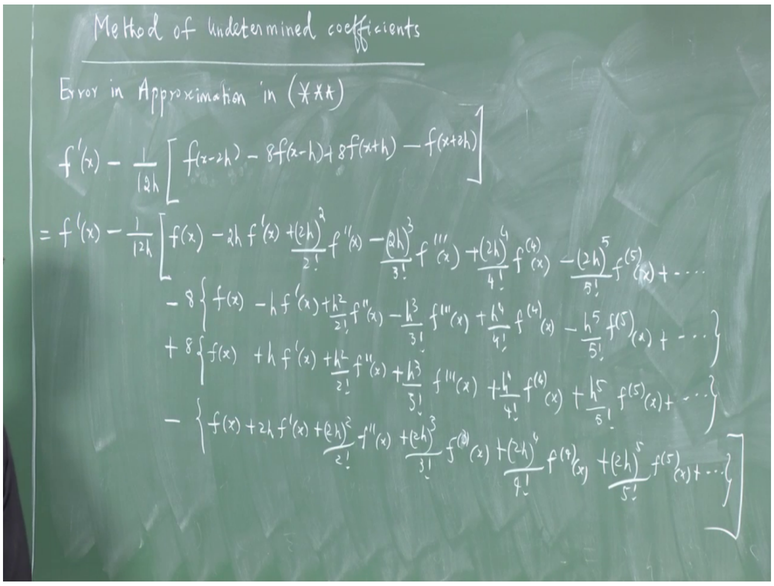


So Error in Approximation in so the error expression is given by f prime (x) minus 1 by 12 h into [ f(x minus 2 h) minus 8into f( x minus h) plus 8 f(x plus h ) and then I have minus f(x plus 2 h)]. So I should compute the difference between f prime and the terms on the right hand side.

So this will be equal to f prime (x minus 1 by 12 h) into let us Taylor's theorem and expand this function f(x minus 2h) so it is f(x) minus 2h into f prime (x) plus (2h) the whole square by factorial 2 into f double prime (x) minus (2h) the whole cube by factorial 3 into f triple prime (x) plus (2h) the whole power 4 by factorial 4 into 4 th derivative of x (minus 2h) the whole power 5 by factorial 5 into fifth derivative at (x).

I can write down some more terms let us stop at this and let us see whether we are able to obtain an expression for the error term. Since I have truncated here this is going to be the error term in expanding f(x minus 2h) about the point x. So I present the error in terms of the 5 th derivative say at 5.

Then the next term is going to be minus 8 times or I can take it to the x because I do not know whether I should truncate it here or I should take more number of terms so I shall just write this and say it as etc. And then continue to write down this term which is minus 8 times { f(x) minus h f prime (x) plus h square by factorial 2 plus f double prime (x) minus h cube by factorial 3 f triple prime (x) plus h power 4 by factorial 4 into fourth derivative at x minus h power 5 by factorial 5 into fifth derivative of (x) plus etc}.

Then I shall write down the next term plus 8 into { f(x) plus h f prime (x) plus h square by factorial 2 f double prime (x) minus h cube by factorial 3 f triple prime (x) plus h power 4 by factorial 4 into fourth derivative at x then minus h power 5 by factorial 5 this is f(x plush) so all the terms will have positive signs fifth derivative of x plus etc}.

And then  I have the last term which is minus f(x plus 2h) so it is f (x plus 2h) f prime x plus (2h) the whole square by factorial 2 f double prime x plus (2h) the whole cube by factorial 3 into the third derivative  at x plus (2h) the whole power 4 by factorial 4 into fourth derivative plus (2h) power 5 by factorial 5 into the fifth derivative at x plus etc}].

So we have written down all these terms using Taylor expansion all the other derivatives which appear in the expansion  have coefficient be 0 the fifth derivative has its coefficient to be non zero.

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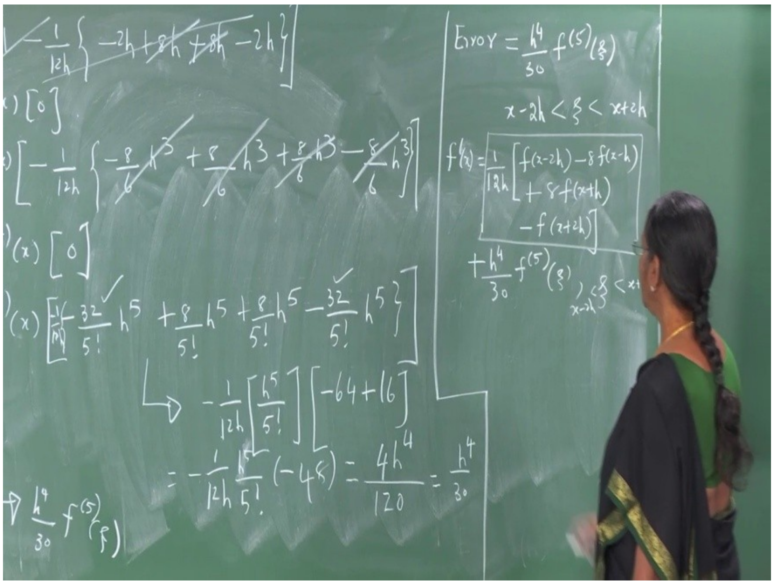

And the error is given by h power 4 by 30 into the fifth derivative evaluated at Psi. Where does this Psi lie It lies between x minus 2h and the x plus 2h And so we have a numerical differentiation formula for f prime (x) given by  f prime (x) is 1 by 12 h into f at (x minus 2h) minus 8 f(x minus h) plus 8 f at (x plus h) and the last term its minus f at(x plus 2h) and the error term is h power 4 by 30 into the fifth derivative at 5 for 5 lying between (x minus 2h) and (x plus 2h).

 So f prime (x) can be estimated in terms of the values of the function at these points which will be given to us in table of values

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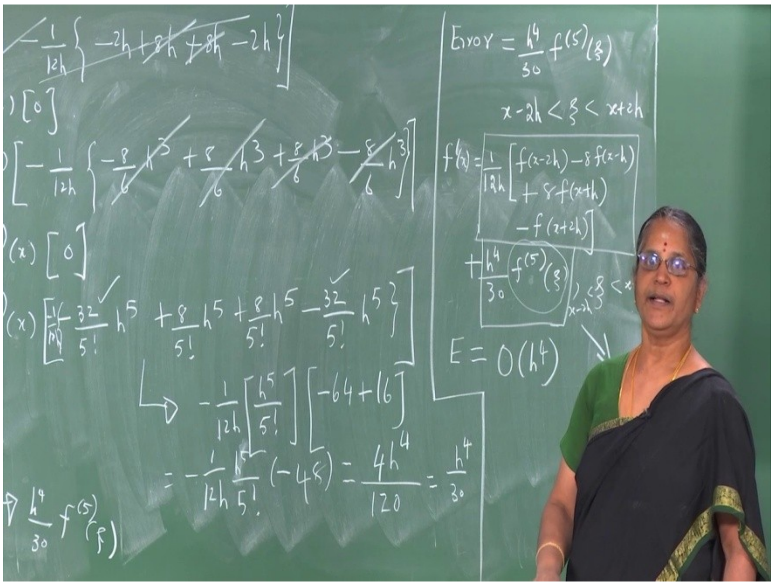


And error term is given by this expression so the error is of order of (h to the power of 4) and the factor which appears here is namely the first order derivative tells you the class of function f for which the first derivative can be estimated using this formula namely f f prime f double prime f triple prime  f four prime has been such that they are continuous in the interval (x minus 2h) to (x plus 2h). And the fifth derivative must exist in the open interval (x minus 2h) to (x plus 2h).

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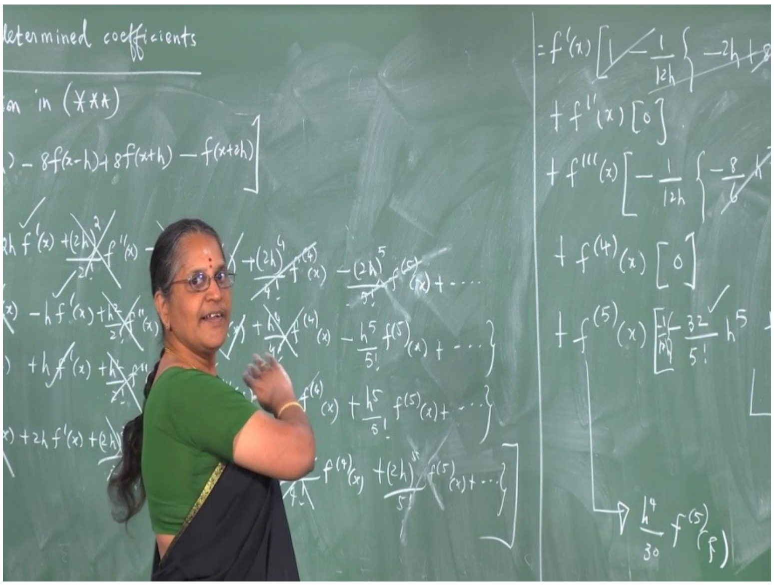

So you get an information about the class of functions for which the first derivative can be approximated by the first term from the expression in the error term. So we have now used method of undetermined coefficients. We shall just recall what it is? We propose a method for approximating a derivative of the function and then we say that this method must be exact for polynomials upto certain degree namely we enforce the conditions in such a way that there are as many conditions as we have unknowns appearing in the proposed formula.

And so depending on that we make the method exact upto polynomials of certain degree and determine these unknown coefficients and compute the error that is incurred in that proposed method Which gives us the order of accuracy of the method and in addition it provides for what class of functions we can use the proposed method to estimate that particular derivative which has been given or which has been obtained using this numerical differentiation method.

So we have a number of such formulas on numerical differentiation methods for evaluating order derivatives which can be derived by proceeding in the manner in which we have obtained this particular method So I shall give you one or two such methods and you can try to work out the details you are (())(19:45).

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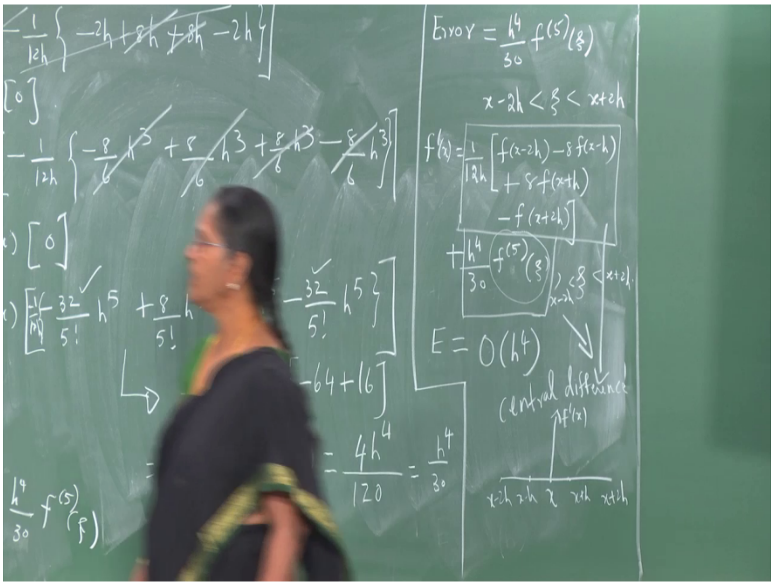


So another observation on this method is that this method is to avoid a simple difference approximation for the reason that you have been able to estimate a derivative at this point x in terms of the function values at x minus h x minus 2h x plus h and x plus 2h which lie symmetrically on either side of this point x. So this method is known as difference approximation method.

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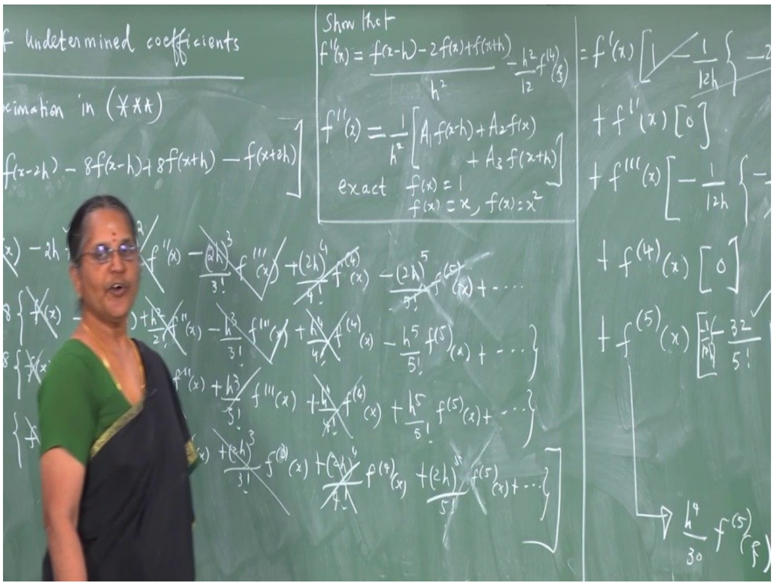


So as I said I shall give you one or two such methods And I would like you to obtain those methods like working out the details. So show that the second derivative f double prime (x) can be approximated by 35. We have already derived this using Taylor Expansion earlier and we have showed this result. But now I want you to obtain this method by the method of undetermined questions.

So how do you start You say that you proposed a method which is the form 1 by h square into A 1 into f (x minus h) plus A 2 into f(x) plus A 3 into f ( x plus h) which is again a central difference formula because it gives you the derivative at x in terms of the function values and either side of x along with value at x Its a central difference scheme.

So how will you determine A 1 A 2 A 3 There are three constants so you require three conditions so you determine A 1 A 2 A 3 in such a way that the method is exact for polynomials of degree 1 mainly constant polynomials sorry polynomials of degree 0 mainly constant polynomials for a first degree polynomial and second degree polynomial.

So you make this method exact for polynomial sub degree upto 2 and this will give you three conditions and if you use these three conditions to evaluate what are A 1, A 2, A 3. And once you obtain the formula you will compute the truncation error in the approximation of that method and approximation of that derivative in a way similar to this.

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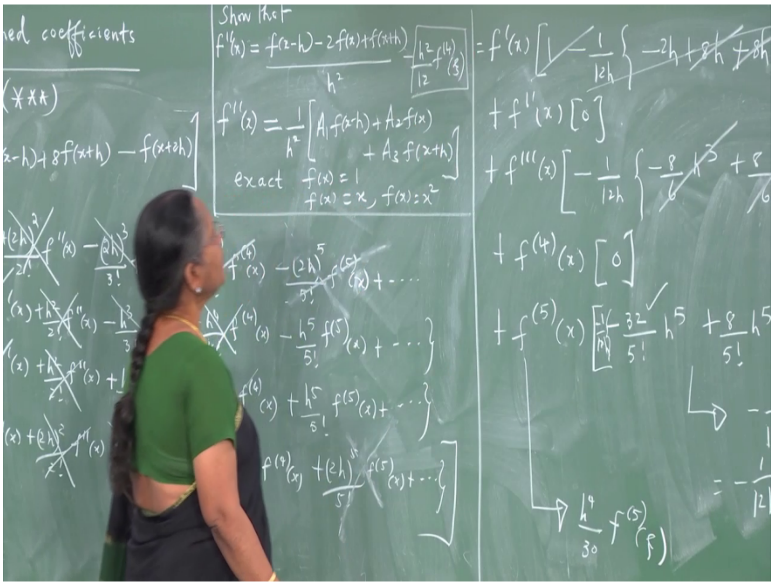


And then show that the error is this So your method is valid for a class of functions f such that the fourth derivative exists in a local interval (x minus h) to ( x plus h) and this is h square by 12 into the fourth derivative so half of function f  such that the fourth derivative exists in (x minus h ) to ( x plus h) in open interval And f f prime  f double prime f triple prime exists in our continuous in the closed interval (x minus h) to ( x plus h) and the error is of order of h square So try to derive this method.

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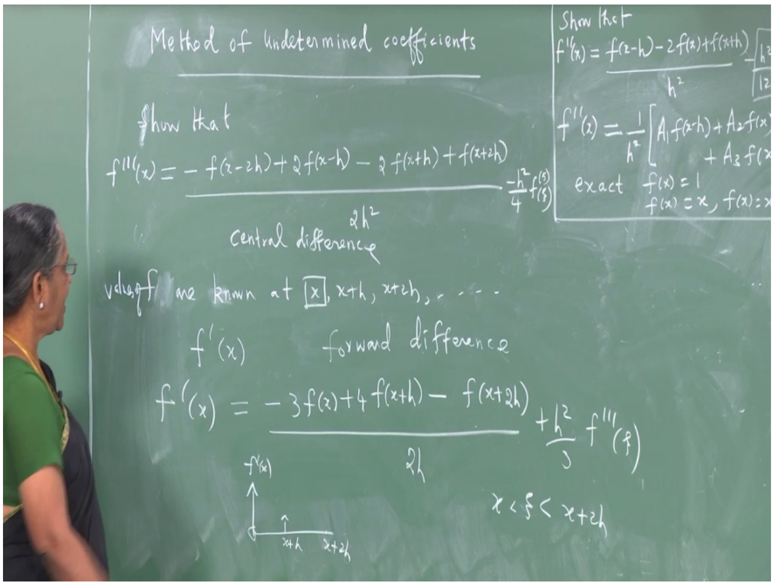

So I shall give you another example to show that f triple prime (x) the third derivative can be given by f( x minus 2h) minus twice f (x minus h) minus twice f( x plus h) plus f(x plus 2h) divided by 2 h square minus h square by 4 into the first derivative at Psi. Which is again a central difference formula for third derivative at x which involves information of the function values at ( x minus h) ( x minus 2h) and ( x plus h ) and ( x plus 2h).

Suppose you require numerical differentiation methods from which you have to compute the various order derivative at one end point of the set of information that is given to you. We need if suppose the function values f(x) values of f are known at x x plus h x plus 2h etc and you require say the first derivative at this end point x of a set of values which are given to you then you have changed this formula using forward differences mainly workout the details and show at f prime at this end point and the estimated by minus thrice f(x) plus 4 times f(x plush) minus f (x plus 2h) by 2h.

And the error involved is of order of h square and the term f triple prime (Psi) indicates that it must exists where in the interval x to x plus 2h with f f prime f double prime continuous in the closed interval x to x plus 2h. So you observe that the derivative at this end point is required and it is given in terms of the function values at x the function values at x plus h and the value at x plus 2h So it involves the function values at y to the right of x.

So it is called forward difference approximation to the derivative f dash (x). So you can derive by method of undetermined coefficients Either forward difference approximations and analogously backward difference approximations in terms of the values to the left of x mainly values at x minus h x minus 2h and so on for various order derivatives. Or using central difference approximations for any order derivative.

So the method of undetermined coefficient is very useful when you have information about the function values at affect of point which are equally spaced and the estimate for various order derivatives can be computed either using forward difference formulas or central difference formulas or backward difference formulas.

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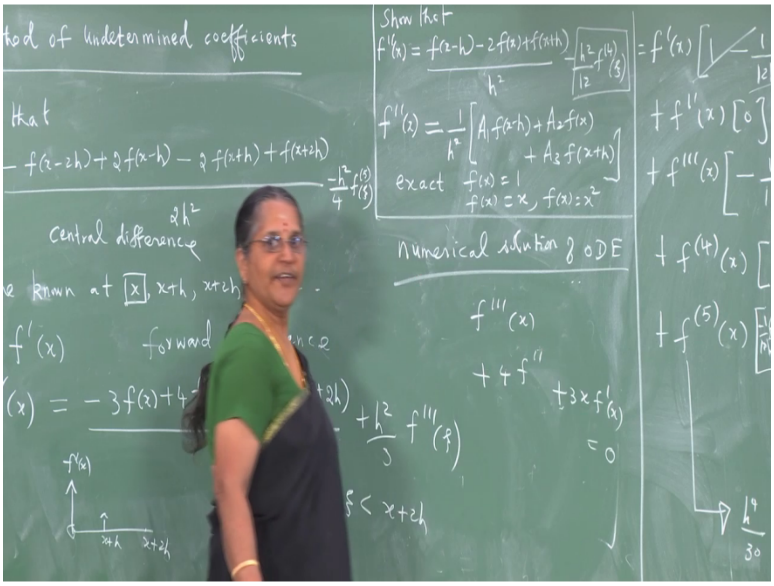


The natural question comes to you where are they useful to us. Why are we deriving these numerical differentiation methods. These formulas are going to be very useful when we take up for the numerical solution of differential equations either ordinary differential equations or partial differential equations but in the case of partial differential equations we will have to obtain an approximation for a partial derivative.

But what we have done in this course or in todays class will be very useful for us in numerical solution of ordinary differential equation. How was it useful Suppose it involves say third order derivative or the second order derivative or some 3x times a first order derivatives say suppose you will have to solve an equation of this form.

Then you are unable to solve any of the techniques that is known to you so in some interval say [01] or some interval then you can approximate these derivatives by means of the finite difference approximations namely the numerical differentiation methods either throughout by forward differences or throughout by central differences or by backward differences.

So that you know what is the order of accuracy of the method that you propose to solve this differential equation numerically. So once you have replaced the derivatives by means of their finite difference approximations you need to solve the unknown value at a set of discrete points namely the points x x minus h x minus 2h or x plus h x plus 2h and so on.

So you will end up with a system of algebraic equations and then solve these by the methods which are available for solving a system of algebraic equations. You arrive at a solution at a set discrete points So you get a numerical solution of the ordinary differential equations and the numerical differential techniques are methods but we develop are many useful in solving or in obtaining the numerical solution of ordinary differential equations. So we shall continue with some more methods for obtaining numerical differentiation formulas in the next class.