

**Elementary Numerical Analysis**  
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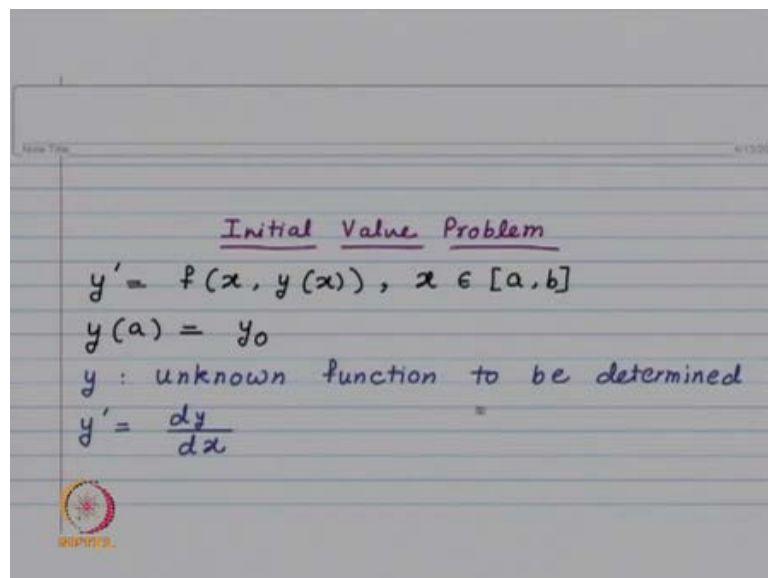
**Lecture No. # 32**  
**Multi-Step Methods**

We are considering approximate solution of initial value problem. So, we have already considered Euler's method and the local discretization error in the Euler's method is  $h^3$  and the total error it is of the order of  $h^2$ .

So, now today we are going to consider in the Euler's method. We had the local discretization error to be  $h^2$ . Now, today, we are going to consider Runge-Kutta method of order two and we will derive this method along with the error. And then I will state Runge-Kutta method of order 4, after that we will consider multi step formulae for example, Adams Bashforth method.

So, we are looking at the initial value problem.

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Initial Value Problem

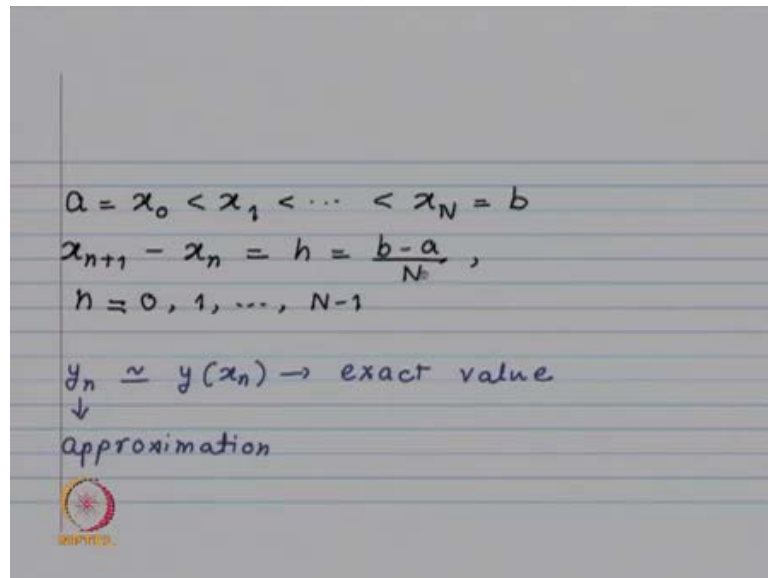
$$y' = f(x, y(x)), x \in [a, b]$$
$$y(a) = y_0$$

$y$  : unknown function to be determined

$$y' = \frac{dy}{dx}$$

$y'$  is equal to  $f$  of  $x$ ,  $y(x)$ ,  $x$  belonging to  $a, b$ , with initial value  $y(a) = y_0$ . Given  $y$  is the unknown function to be determined, and the notation is  $y'$  is equal to  $\frac{dy}{dx}$ . What we do is, we sub divide this interval  $a, b$  into  $n$  equal part.

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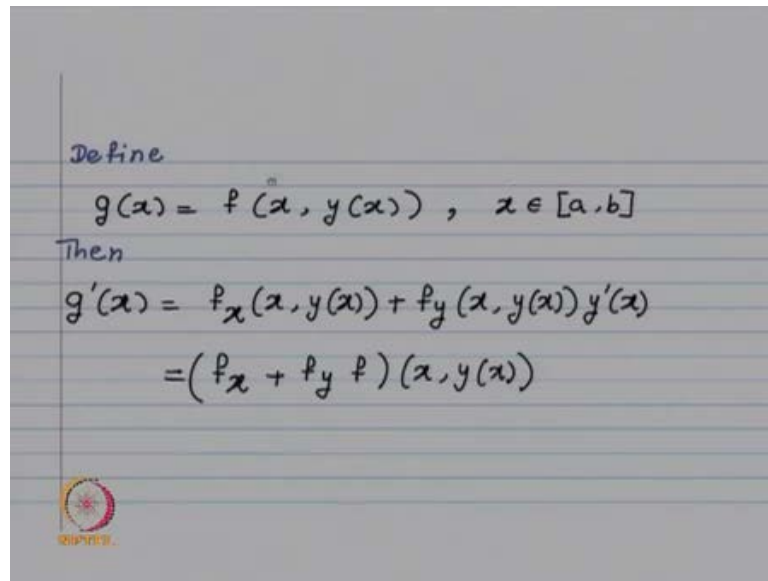

$$a = x_0 < x_1 < \dots < x_N = b$$
$$x_{n+1} - x_n = h = \frac{b-a}{N},$$
$$n = 0, 1, \dots, N-1$$

$y_n \approx y(x_n) \rightarrow$  exact value  
 $\downarrow$   
approximation

So,  $a$  is equal to  $x_0$ , less than  $x_1$ , less than  $x_n$  is equal to  $b$ .

Each sub interval is of length of  $h$ , which is going to be equal to,  $b$  minus  $a$  divided by capital  $N$ , at  $x_n$  is the exact value of the unknown function, and  $y_n$  is going to be an approximation to this. So, our aim is to find approximation to  $y$  at  $x_n$  at these  $n$  plus 1 points.

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Define

$$g(x) = f(x, y(x)), \quad x \in [a, b]$$

Then

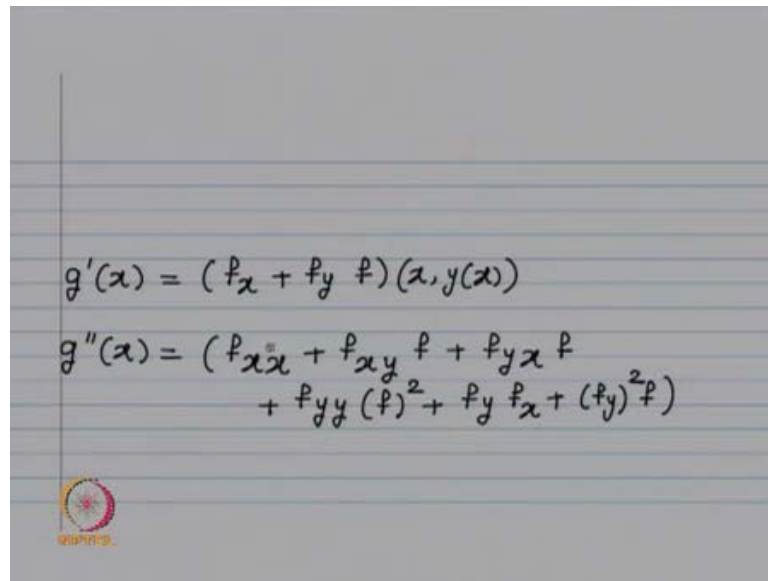
$$g'(x) = f_x(x, y(x)) + f_y(x, y(x))y'(x)$$
$$= (f_x + f_y f')(x, y(x))$$

The right hand side function it is  $f$  is a function of  $x$  and  $y$  and  $y$  is a function of  $x$ . So, we have got this function  $g$   $x$  defined on interval  $a$   $b$  when we want to calculate the derivative of  $g$ . So, that is going to be equal to  $g$  dash  $x$  is equal to by chain rule partial derivative of  $f$  with respect to  $x$  plus partial derivative of  $f$  with respect to  $y$  and ,now  $y$  is a function of  $x$ . So, it is  $y$  dash of  $x$ .

We know that  $y$  dash is equal to  $f$ . So  $g$  dash  $x$  is going to be  $f_x$  plus  $f_y$  into  $f$  evaluated at  $x$   $y$ . So, this is the first derivative .Now let us look at the second derivative. So, the second derivative, we have calculated the first derivative ,in the first derivative we have got partial derivatives of  $f$  with respect to  $x$  partial derivative of  $f$  with respect to  $y$  and the function  $f$ .

Function  $f$  partial derivative with respect to  $x$  and partial derivative with respect to  $y$  ,they are going to be function of  $x$  and  $y$ . So, when we want to calculate the second derivative, we will again apply chain rule and then when you are considering partial derivative with respect to  $I$  into  $y$  dash, we will be substituting for  $y$  dash is equal to  $f$ . So, taking these things into consideration the second derivative of  $g$  is going to be given by

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$$g'(x) = (f_x + f_y f')(x, y(x))$$
$$g''(x) = (f_{xx} + f_{xy} f' + f_{yx} f' + f_{yy} (f')^2 + f_y f'_x + (f'_y)^2 f')(x, y(x))$$

$g''(x)$  is  $f_{xx}$  then  $f_{xy}$  partial derivative of  $f_x$  with respect to  $y$  multiplied by  $y'$ . So, that is going to be equal to  $f'$ .

So, this is derivative of  $f_x$  with respect to  $x$  these 2 terms, now we will be applying product rule. So, here  $f_{yx}$  into  $f'$  then  $f_{xy}$  into  $y'$ , that is  $f'$  and then there is 1  $f'$  here. So, it is  $f_{yy} (f')^2$  then  $f_y$  into  $f'_x$  plus  $f_y f'_x$ . So, that will be  $f_y$  square into  $y'$  that is  $f'$ .

And all these functions they will be evaluated at  $x, y(x)$ . So, we have calculated the derivatives of the right hand side with respect to  $x$ , now we are going to look at the

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Runge - Kutta Method of order 2

$$y(x_{n+1}) = y(x_n) + h y'(x_n) + \frac{h^2}{2} y''(x_n) + \frac{h^3}{6} y'''(x_n) + O(h^4) \dots (1)$$
$$y_{n+1} = y_n + a k_1 + b k_2, \dots (2)$$
$$k_1 = h f(x_n, y_n),$$
$$k_2 = h f(x_n + \alpha h, y_n + \beta k_1)$$

Taylor series expansion, for unknown function  $y$ . So, value of  $y$  at  $x_{n+1}$ , will be equal to,  $y(x_n) + h y'(x_n) + \frac{h^2}{2} y''(x_n) + \frac{h^3}{6} y'''(x_n) + \dots$

So, this is the Taylor series expansion. Suppose I truncate this series, by keeping the first three terms. Then we are going to have the local discretization error, to be of the order of  $h^3$ . The formula which you obtain involves the function  $f$  and its partial derivatives with respect to  $x$  and with respect to  $y$ .

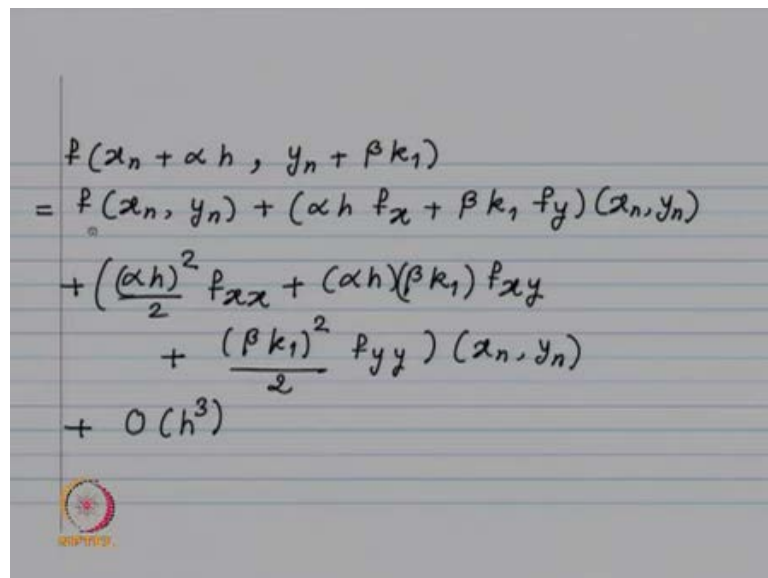
What we want to do is get a formula which involves only function  $f$  and not its partial derivative. So, we try to determine  $y_{n+1}$  to be equal to  $y_n + a k_1 + b k_2$  where  $k_1$  is going to be  $h f(x_n, y_n)$ .

$k_2$  is going to be  $h f(x_n + \alpha h, y_n + \beta k_1)$ . So, the constants  $a, b, \alpha$  and  $\beta$  they are at our disposal, we want to determine these constants. So, that the first 3 terms they are going to match here, you have got  $y'$  at  $x_n$ ,  $y'$  is equal to  $f$ . So, you have got a term  $f(x_n, y_n)$  we also want to match the term which contains  $h^2$  and then the formula which we will obtain will have a local discretization error to be of the order of the  $h^3$ .

So, the way we are going to do this is we have got,  $f(x_n + \alpha h, y_n + \beta k_1)$  use Taylor series expansion for function of two variables. So, this  $f(x_n + \alpha h, y_n + \beta k_1)$

$x_n + \beta k_1$  will be equal to  $f(x_n, y_n + \alpha h)$  and then partial derivative of  $f$  with respect to  $x$  evaluated at  $x_n, y_n + \beta k_1$  partial derivative of  $f$  with respect to  $y$  evaluated at  $x_n, y_n$ .

When we look at the Taylor series expansion for  $y$  at  $x_n + 1$ , that also involves the terms  $f_x, f_y$ . So, then we will be able to compare the terms and determine  $\alpha$  and  $\beta$ . So, that the constant term, the term which contains  $h$  and the term which contains  $h^2$ , they are going to match and that will give us a formula which involves only the function  $f$ , but the local discretization error is of the order of  $h^3$ . So, let us write down the Taylor series expansion for function of two variables  $f(x_n + \alpha h, y_n + \beta k_1)$  (Refer Slide Time: 08:39)



$$\begin{aligned}
 & f(x_n + \alpha h, y_n + \beta k_1) \\
 &= f(x_n, y_n) + (\alpha h f_x + \beta k_1 f_y)(x_n, y_n) \\
 &+ \left( \frac{(\alpha h)^2}{2} f_{xx} + (\alpha h)(\beta k_1) f_{xy} \right. \\
 &\quad \left. + \frac{(\beta k_1)^2}{2} f_{yy} \right)(x_n, y_n) \\
 &+ O(h^3)
 \end{aligned}$$

The Taylor series expansion is  $f(x_n, y_n + \alpha h)$  into partial derivative of  $f$  with respect to  $x$  plus  $\beta k_1$  into partial derivative of  $f$  with respect to  $y$ . All the functions to be evaluated at  $x_n, y_n$ , the next term will be  $\alpha h^2$  by 2, the second order of partial derivative with respect to  $x$ .

Plus  $\alpha h \beta k_1 f_{xy}$  plus  $\beta k_1^2$  by 2  $f_{yy}$  evaluated at  $x_n, y_n$  plus term of the order of  $h^3$ . So, this is the Taylor series expansion for the function of two variables now this is the

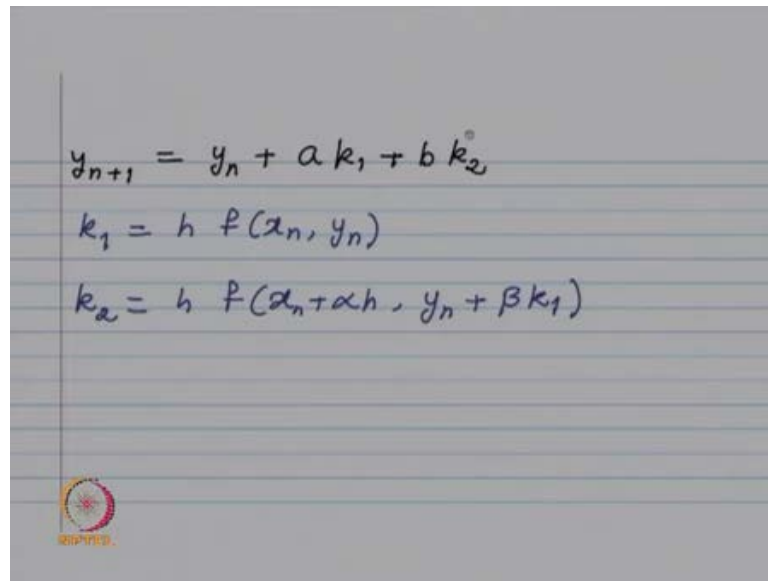
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$$\begin{aligned}
 y(x_{n+1}) &= y(x_n) + h y'(x_n) + \frac{h^2}{2} y''(x_n) \\
 &\quad + \frac{h^3}{6} y'''(x_n) + O(h^4) \\
 &= y(x_n) + h f(x_n, y_n) + \frac{h^2}{2} (f_{xx} + f_y \cdot f) \\
 &\quad + \frac{h^3}{6} (f_{xx} + 2 f_{xy} f + f_{yy} f^2 \\
 &\quad \quad + f_y f_x + (f_y)^2 f)(x_n, y(x_n))
 \end{aligned}$$

Taylor series expansion for the unknown function  $y$   $y'$  is  $f$   $y''$  is nothing, but derivative of this  $f$ . So, that is going to be equal to  $f_x$  plus  $f_y$  into  $f$  plus  $h^3$  by 6. Now derivative of this, and we have seen the derivative of this to be equal to  $f_{xx}$  plus two times  $f_{xy} f$  assuming that the mixed partial derivatives they are equal; that means,  $f_{xy}$  is equal to  $f_{yx}$  plus  $f_{yy} f^2$ , plus  $f_y$  into  $f_x$ , plus  $f_y$  square into  $f$  at  $x_n$  and then  $y$  at  $x_n$ .

So, here this  $h^2$  by 2 to this function also you will be evaluated at  $x_n, y(x_n)$  and same thing here. So, our  $y_{n+1}$  the formula is going to be of this form,  $y_n$  plus  $h f(x_n, y_n)$  plus  $\frac{h^2}{2} (f_{xx} + f_y f)$  plus  $\frac{h^3}{6} (f_{xx} + 2 f_{xy} f + f_{yy} f^2 + f_y f_x + (f_y)^2 f)(x_n, y(x_n))$ , then we have seen this to be the Taylor series expansion. So, this Taylor series expansion

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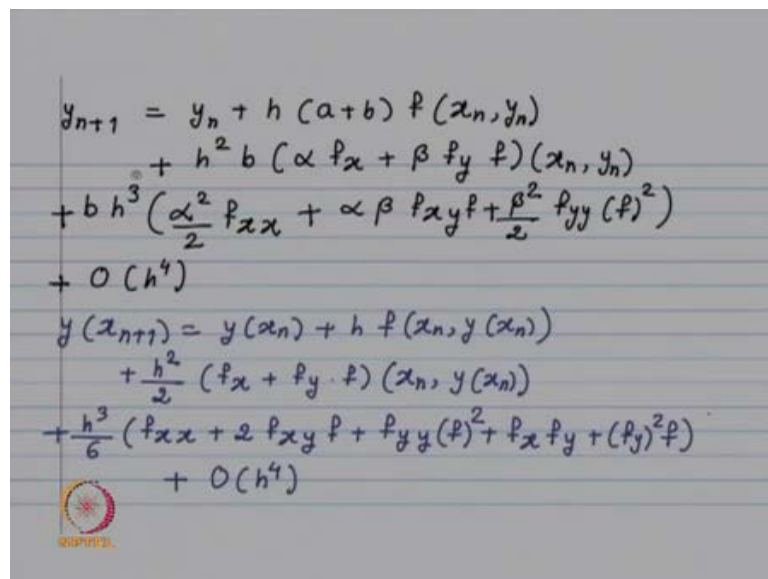
Handwritten equations on a lined background:

$$y_{n+1} = y_n + a k_1 + b k_2$$
$$k_1 = h f(x_n, y_n)$$
$$k_2 = h f(x_n + \alpha h, y_n + \beta k_1)$$

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we are going to substitute here

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Handwritten Taylor series expansion on a lined background:

$$y_{n+1} = y_n + h(a+b) f(x_n, y_n)$$
$$+ h^2 b (\alpha f_x + \beta f_y f)(x_n, y_n)$$
$$+ b h^3 \left( \frac{\alpha^2}{2} f_{xx} + \alpha \beta f_{xy} f + \frac{\beta^2}{2} f_{yy} (f)^2 \right)$$
$$+ O(h^4)$$
$$y(x_{n+1}) = y(x_n) + h f(x_n, y(x_n))$$
$$+ \frac{h^2}{2} (f_x + f_y \cdot f)(x_n, y(x_n))$$
$$+ \frac{h^3}{6} (f_{xx} + 2 f_{xy} f + f_{yy} (f)^2 + f_x f_y + (f_y)^2 f)$$
$$+ O(h^4)$$

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and then we get  $y_{n+1}$  is equal to  $y_n$  plus  $h$  times  $a + b f$  of  $x_n, y_n$ , because our  $y_{n+1}$  is  $y_n$  plus  $h$  times  $k_1$  plus  $a$  times  $k_1$  plus  $b$  times  $k_2$ .

Then. So, we have



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$$y_{n+1} = y_n + a k_1 + b k_2$$

$$k_1 = h f(x_n, y_n)$$

$$k_2 = h f(x_n + \alpha h, y_n + \beta k_1)$$

↓  
Taylor series exp.

$y_{n+1}$  is equal to  $y_n$  plus  $a k_1$  plus  $b k_2$ .  $k_1$  is  $h$  times  $f$  of  $x_n, y_n$ .  $k_2$  is  $h$  times  $f$  of  $x_n + \alpha h, y_n + \beta k_1$ , for this we write Taylor series expansion.

And then when we substitute in this formula. So, you are going to have  $h$  times  $a$  of  $f$  plus from here you will get  $b$  of  $f$ . So, that is why we have got  $y_{n+1}$

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$$y_{n+1} = y_n + h(a+b) f(x_n, y_n)$$

$$+ h^2 b (\alpha f_x + \beta f_y f)(x_n, y_n)$$

$$+ b h^3 \left( \frac{\alpha^2}{2} f_{xx} + \alpha \beta f_{xy} f + \frac{\beta^2}{2} f_{yy} (f)^2 \right)$$

$$+ O(h^4)$$

$$y(x_{n+1}) = y(x_n) + h f(x_n, y(x_n))$$

$$+ \frac{h^2}{2} (f_x + f_y \cdot f)(x_n, y(x_n))$$

$$+ \frac{h^3}{6} (f_{xx} + 2 f_{xy} f + f_{yy} (f)^2 + f_x f_y + (f_y)^2 f)$$

$$+ O(h^4)$$

is equal to  $y_n$ , plus  $h$  times  $a$  plus  $b$ ,  $f$  of  $x_n, y_n$  plus  $h$  square times  $b$  alpha  $f_x$  plus beta  $f_y$  into  $f$  of  $x_n, y_n$ , plus the coefficient of  $h$  cube is going to be this term plus term of the order of  $h$  raise to 4..

So, it is just substitute the Taylor series expansion and then write down what you get then this is our Taylor series expansion .For y at x n plus 1 ,we are going to compare these 2. We are going to neglect the error between y x n and y n ,we are going to look at only local discretization error.

That means you have calculated approximation y n now from y n I am going to y n plus one. So, at this particular step for going from x n to x n plus 1 ,whatever is the error that is our local discretization error and that we are trying to determine. So, we will assume that y at x n is equal to y n. So, with this assumption

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The image shows a handwritten derivation on lined paper. It compares two expressions for  $y_{n+1}$ . The first expression is a Taylor series expansion of  $y_{n+1}$  around  $(x_n, y_n)$ . The second expression is a Taylor series expansion of  $y(x_{n+1})$  around  $(x_n, y(x_n))$ . The two expressions are compared term by term to find conditions for matching.

$$\begin{aligned}
 y_{n+1} &= y_n + h(a+b) f(x_n, y_n) \\
 &\quad + h^2 b (\alpha f_x + \beta f_y \cdot f)(x_n, y_n) \\
 &\quad + b h^3 \left( \frac{\alpha^2}{2} f_{xx} + \alpha \beta f_{xy} f + \frac{\beta^2}{2} f_{yy} (f)^2 \right) \\
 &\quad + O(h^4) \\
 y(x_{n+1}) &= y(x_n) + h f(x_n, y(x_n)) \\
 &\quad + \frac{h^2}{2} (f_x + f_y \cdot f)(x_n, y(x_n)) \\
 &\quad + \frac{h^3}{6} (f_{xx} + 2 f_{xy} f + f_{yy} (f)^2 + f_x f_y + (f_y)^2 f) \\
 &\quad + O(h^4)
 \end{aligned}$$

When you compare these 2 y n is going to be same as y at x n. So, the constant terms match then here, you have h times f of x n y x n, which is same as f of x n y n and here you have f of x n y n.

So, if we want these two terms to match our a plus b should be equal to 1. So, we get the first condition on a and b ,that a plus b should be equal to 1. Now look at the next term, you have got h square ,here h square here, then here you have f x plus f y f divided by 2 and here you have got b alpha f x plus b beta f y f x n y n. So, if I want this term and this term to match .Then what I should do is b or into alpha should be equal to 1 by 2 b into beta should be equal to 1 by 2.

So, we have  $a + b = 1$ ,  $b\alpha = 1/2$ ,  $b\beta = 1/2$ . So, thus if I choose my  $a, b, \alpha$  and  $\beta$  such that  $a + b = 1$ ,  $b\alpha = 1/2$ ,  $b\beta = 1/2$ .

Then constant term, the term which contains  $h$  and the term which contains  $h^2$  they are going to match with the assumption that  $y_{n+1} = y_n + hf(x_n, y_n)$ . Now we have got four constants, we have got one more say degree of freedom at our disposal like, I can impose one more condition.

Now, whether by imposing that condition, if I can also match the coefficient of  $h^3$  then that will be good, because then our local discretization error will be of the order of  $h^4$ . But no matter how you choose your  $a, b, \alpha, \beta$ , it will not be possible because when you look at  $y_{n+1}$ .

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The image shows a handwritten derivation on lined paper. It compares the Taylor expansion of the exact solution  $y(x_{n+1})$  with the Runge-Kutta method approximation  $y_{n+1}$ .

The Runge-Kutta approximation is given as:

$$y_{n+1} = y_n + h(a+b)f(x_n, y_n) + h^2 b(\alpha f_x + \beta f_y f)(x_n, y_n) + b h^3 \left( \frac{\alpha^2}{2} f_{xx} + \alpha\beta f_{xy} f + \frac{\beta^2}{2} f_{yy} (f)^2 \right) + O(h^4)$$

The Taylor expansion of the exact solution is given as:

$$y(x_{n+1}) = y(x_n) + h f(x_n, y(x_n)) + \frac{h^2}{2} (f_x + f_y \cdot f)(x_n, y(x_n)) + \frac{h^3}{6} (f_{xx} + 2 f_{xy} f + f_{yy} (f)^2 + f_x f_y + (f_y)^2 f) + O(h^4)$$


In the coefficient of  $h^3$  you have got  $f_{xx}, f_{xy} f$ , and then  $f_{yy} (f)^2$ . Whereas, in  $y_{n+1}$  you have got these three terms and in addition  $f_x f_y$  and  $(f_y)^2 f$ . So, no matter which way you choose your  $a, b, \alpha, \beta$ , you cannot hope to match the coefficients of  $h^3$ .

Because of the presence of these. So, **So**, now, we have got the condition

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$$\begin{aligned}y_{n+1} &= y_n + a k_1 + b k_2, \\k_1 &= h f(x_n, y_n) \\k_2 &= h f(x_n + \alpha h, y_n + \beta k_1) \\a + b &= 1, \quad b \alpha = \frac{1}{2}, \quad b \beta = \frac{1}{2} \\a = b = \frac{1}{2}, \quad \alpha = \beta &= 1\end{aligned}$$

local discretization error =  $O(h^3)$



a plus b is equal to 1, b alpha is equal to half, b beta is equal to half, four constants and only three conditions. So, there are infinitely many ways of choosing this. So, let us choose which is something symmetric. So, choose a is equal to b is equal to half alpha is equal to beta is equal to 1.

Then the local discretization error is going to be of the order of h cube. So, this is the known as runge-kutta method of order two. What you need to do is evaluate your function f at  $x_n, y_n$ , and then evaluate your function f at  $x_n + h, y_n + k_1$  you have calculated  $k_1$ . So, you calculate that and then you take the mean of these 2 a and is equal to half. So, it is going to be h times f of  $x_n, y_n$  plus h times f of  $x_n + h, y_n + k_1$ , divided by 2.

So, that is the runge-kutta method of order two and local discretization error is of the order of h cube.

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$$\begin{aligned} & y(x_{n+1}) - y_{n+1} \\ &= \frac{h^3}{6} (f_{xx} + 2f_{xy}f + f_{yy}(f)^2 + f_x f_y + (f_y)^2 f) \\ &\quad - \frac{h^3}{4} (f_{xx} + 2f_{xy}f + f_{yy}(f)^2) + O(h^4) \\ &= -\frac{h^3}{12} (f_{xx} + 2f_{xy}f + f_{yy}(f)^2 - 2f_x f_y \\ &\quad \quad \quad - 2(f_y)^2 f) + O(h^4) \end{aligned}$$

So, if I consider the error now  $y(x_{n+1}) - y_{n+1}$ . So, this is the term in  $y$  at  $x_{n+1}$  which contains  $h^3$  the corresponding term in  $y_{n+1}$  which contains  $h^3$  is given by this, I am subtracting and then you have got terms of the order of  $h$  raised to 4. So, this is equal to when you simplify it will be minus  $h^3$  by 12 times.

This factor plus the term of the order of  $h$  raised to 4. So, this is 1 of the undesirable property of Runge-Kutta method, when you look at  $y(x_{n+1}) - y_{n+1}$ . So, we look at the coefficient of  $h^3$ . So, that coefficient of  $h^3$  it is quite complicated and then you have higher order terms.

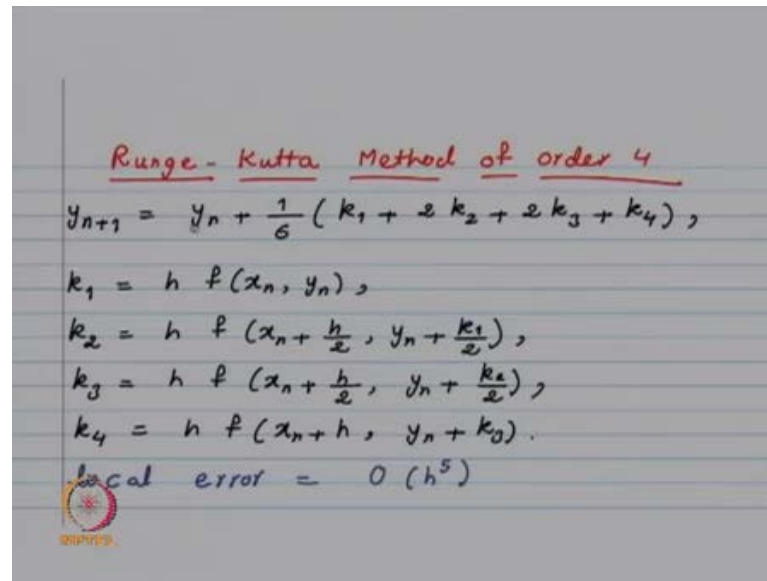
I will talk about this little more in detail when we compare Runge-Kutta methods with other methods. Now what I am going to do is, state Runge-Kutta method of order four whatever technique we have used, we can try to do it for higher order.

Methods like here we had tried to match the coefficients in the Taylor series expansion. For the unknown function  $y$ , which contain the constant terms the term which contain  $h$  and the term which contain  $h^2$ .

Now, in best on a similar principle I can derive a method which is known as Runge-Kutta method of order four. The principle is the same the computations, they become messy. So, let me just state what is Runge-Kutta method of order four.

So, that is

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Runge-Kutta Method of order 4

$$y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4),$$
$$k_1 = h f(x_n, y_n),$$
$$k_2 = h f\left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right),$$
$$k_3 = h f\left(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right),$$
$$k_4 = h f(x_n + h, y_n + k_3).$$

local error =  $O(h^5)$

$y_{n+1}$  is equal to  $y_n$  plus  $\frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$ . So, what is  $k_1$ ?  $k_1$  as before is  $h$  times  $f$  of  $x_n, y_n$ .  $k_2$  is going to be  $h$  times  $f$  of  $x_n + \frac{h}{2}$  and then  $y_n + \frac{k_1}{2}$ . The increment for  $y_n$  is going to be this  $k_1$ , which you have found.  $k_3$  will be  $h$  times  $f$  of  $x_n + \frac{h}{2}$  as before and then  $y_n + \frac{k_2}{2}$  and  $k_4$  is equal to  $h$  times  $f$  of  $x_n + h, y_n + k_3$  you have found here.

It can be proved that the local error is of the order of  $h^5$ . So, we have got now three methods. One is Euler's method, then we have got a Runge-Kutta method of order two and Runge-Kutta method of order four.

For the Euler's method we had  $y_{n+1}$  is equal to  $y_n$  plus  $h$  times  $f$  of  $x_n, y_n$ ; that means, per step there was 1 function evaluation, when you look at Runge-Kutta method of order 2 we have got  $y_{n+1}$  is equal to  $y_n$  plus  $k_1 + k_2$  by 2 where  $k_1$  is  $h$  times  $f$  of  $x_n, y_n$ .  $k_2$  is  $h$  times  $f$  of  $x_n + \frac{h}{2}, y_n + \frac{k_1}{2}$ ; that means, for each step you are evaluating your function twice and then the local discretization error it improved from  $h^2$  to  $h^3$ . So, your function evaluation is doubled, but the local discretization error improves from  $h^2$  to  $h^3$ .

In Runge-Kutta method of order four, you have got  $y_{n+1}$  is equal to  $y_n$  plus  $k_1 + 2k_2 + 2k_3 + k_4$  divided by 6.

For  $k=1, 2, 3, 4$  you need to evaluate function once. So, you have got in all four function evaluations and the local discretization error is improved from  $h^3$  to  $h^5$

Now, these three methods which I have described they are known as single step methods, because in order to evaluate  $y_{n+1}$ , what comes into picture is  $y_n$  using  $y_n$ . You calculate  $k=1$  and then that  $k=1$  gets introduced in  $k=2$  and so on, but they all depend on  $y_n$ . So, these methods they are known as self starting method, because  $y_0$  is given to us that is the condition in the initial value problem the initial condition.

Once you know  $y_0$  using the formulae you can calculate  $y_1$ , then once you have  $y_1$  you can go to  $y_2$  and so on.

So, these are the known as single step methods, and we have calculated or we have evaluated their local discretization error.

Now, these methods these are classical methods. There are methods which are of relatively recent origin in which case instead of this Taylor series expansion, we are going to use numerical quadrature

Now, what we are going to achieve is for example, in Runge-Kutta method we had local discretization error to be  $h^5$  and we had four function evaluation. So, whether I can reduce the function evaluations. So, in the Adams-Bashforth method, we will show that essentially doing only one function evaluation per step, we will achieve the local discretization error to be  $h^5$ . So, then that is very good that instead of four function evaluations we have got only 1 function evaluation. So, you are reducing your work by 1 means it becomes 1 fourth by retaining still the local discretization error to be of the order of  $h^5$ .

Unfortunately there is a trade off because if we had such a method available then Runge-Kutta method would have disappeared, because the methods which we survive those are the ones which are better in some respect. So, here the method which we are going to derive which essentially needs one function evaluation per step.

It will not be self starting; that means, you will need not only  $y_0$ , but you need  $y_1, y_2, y_3$ . So, these are the things that is not such a big disadvantage, but there are also

stability considerations that single step methods they are always stable whereas, the multi step methods they can have stability problems.

So, those things we will be studying in detail. So, . So, now, let us first see what is the principle behind this numerical quadrature.

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Numerical Integration

$$y'(x) = f(x, y(x)) = g(x), x \in [a, b]$$

$$a = x_0 < x_1 < \dots < x_N = b, h = \frac{b-a}{N}$$

$$\int_{x_n}^{x_{n+1}} y'(x) dx = \int_{x_n}^{x_{n+1}} f(x, y(x)) dx$$

$$\parallel$$

$$y(x_{n+1}) - y(x_n)$$

So, we have got our initial value problem .y dash x is equal to f of x y x. Let me write this function f x y x as g x x ,belonging to a b .This is our uniform partition, a to b integrate both the sides between x n to x n plus 1. So, you have integral x n to x n plus 1 y dash x d x is equal to, integral x n to x n plus 1 f of x y x d x or integral x n to x n plus 1 g x d x integration on the left hand side is, y at x n plus 1 minus y at x n. So, if we can evaluate this exactly or if we can integrate this exactly.

Then value of y at x n plus 1 will be equal to y at x n plus, this integral now in general it will not be not be possible to integrate this exactly. So, we use numerical quadrature rule. So, the simplest numerical quadrature rule which we have considered is rectangle rule.

In which case we approximate the given function by a constant polynomial and that constant polynomial is value of your function at the left end point.

So, then we considered also midpoint rule then trapezoidal rule Simpson's rule and so, the other rules we will consider there will be some problem.



So, let us first look at what is the what rectangle rule

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The image shows a handwritten derivation on a lined background. At the top, it is titled "Rectangle Rule." Below the title, the function is expressed as  $g(x) = g(x_n) + g[x_n, x](x - x_n)$ , with the domain  $x \in [x_n, x_{n+1}]$  indicated. The next line shows the integral approximation:  $\int_{x_n}^{x_{n+1}} g(x) dx \simeq h g(x_n)$ . The error term is then derived as  $\text{Error} = \int_{x_n}^{x_{n+1}} g[x_n, x](x - x_n) dx$ , which is simplified to  $= \frac{g'(c_n) h^2}{2}$ . A small logo is visible in the bottom left corner of the slide.

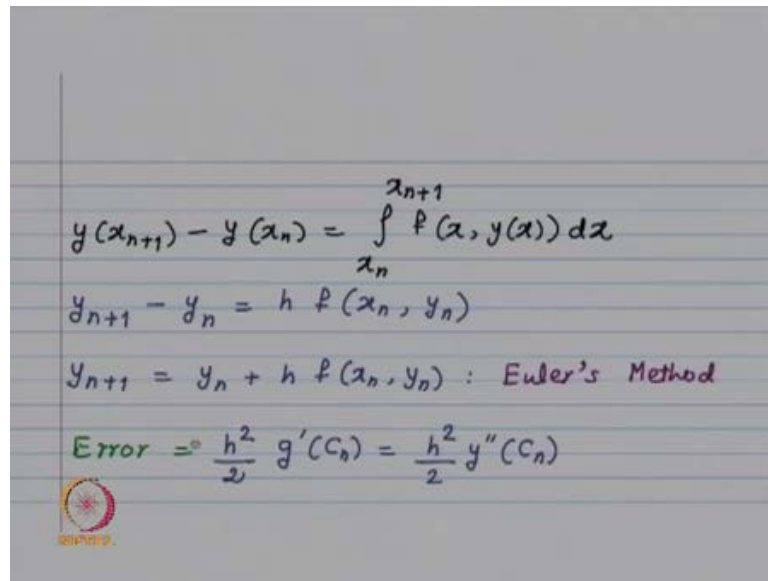
what it gives. So, we have  $g(x)$  that is our function  $f(x, y, x)$  is equal to  $g(x_n)$  and this is the error term divided differences of  $g$  based on,  $x_n$  into  $x$  minus  $x_n$  integral  $x_n$  to  $x_{n+1}$  plus  $1$   $g(x) dx$  is approximately equal to  $h$  times  $g(x_n)$ , the error is given by integral  $x_n$  to  $x_{n+1}$ .

Divided difference  $x$  minus  $x_n$   $dx$  the divided difference is continuous function provided your  $y$  is sufficiently differentiable.

So, this is continuous  $x$  minus  $x_n$  will be bigger than or equal to  $0$ . On the interval  $x_n$  to  $x_{n+1}$ . So, you can use mean value theorem for integrals take this out, and then replace it by  $g'(c_n)$ .

Integral  $x_n$  to  $x_{n+1}$   $x$  minus  $x_n$   $dx$  will be  $x_{n+1} - x_n$  square divided by  $2$ ; that means,  $h^2$  by  $2$ . So, this is the rectangle rule

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The image shows a handwritten derivation of Euler's method on lined paper. The equations are as follows:

$$y(x_{n+1}) - y(x_n) = \int_{x_n}^{x_{n+1}} f(x, y(x)) dx$$
$$y_{n+1} - y_n = h f(x_n, y_n)$$
$$y_{n+1} = y_n + h f(x_n, y_n) : \text{Euler's Method}$$
$$\text{Error} = \frac{h^2}{2} g'(c_n) = \frac{h^2}{2} y''(c_n)$$

A small logo is visible in the bottom left corner of the paper.

and then  $y$  at  $x_{n+1}$  minus  $y$  at  $x_n$  is equal to the integral from  $x_n$  to  $x_{n+1}$  of  $f(x, y(x)) dx$ . This is the equation satisfied by the unknown solution  $y$ . When you apply numerical quadrature rectangle rule to the right hand side you are going to have  $y_{n+1} - y_n$  where  $y_{n+1}$  is approximation to  $y$  at  $x_{n+1}$ .

So,  $y_{n+1} - y_n$  is equal to  $h$  times  $f(x_n, y_n)$ ; that means,  $h$  times  $f$  of  $x_n, y_n$  this is nothing, but our Euler's method.

And the error is  $\frac{h^2}{2} g'(c_n)$  which is same as  $\frac{h^2}{2} y''(c_n)$ . So, now, the rectangle rule gives us back the Euler's method.

So, when we derived Euler's method, what we did was we looked at the Taylor series expansion for, by truncated it keeping only one term or two terms we had kept and that gives us Euler's method.

Now, the another way of looking at Euler's method is apply numerical quadrature to the right hand side, use rectangle rule and then we get Euler's method.

Now, next method is midpoint rule. So, in the midpoint rule what we will be doing will be looking at the midpoint of interval  $x_n$  to  $x_{n+1}$  and then evaluating your function  $f$  at that midpoint.

So, remember you we had

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$$\int_a^b f(x) dx \approx \frac{b-a}{2} f\left(\frac{a+b}{2}\right)$$

Midpoint rule.

$$\int_{x_n}^{x_{n+1}} f(x, y(x)) dx \approx h f\left(\frac{x_n + x_{n+1}}{2}, \frac{y_n + y_{n+1}}{2}\right)$$

integral  $\int_a^b f(x) dx$  to be approximately equal to  $\frac{b-a}{2} f\left(\frac{a+b}{2}\right)$  or the  $\frac{b-a}{2}$  times  $f$  of  $\frac{a+b}{2}$ . So, this is the midpoint rule.

Now, if you consider integral  $\int_{x_n}^{x_{n+1}} f(x, y(x)) dx$ . This will be approximately equal to  $h f\left(\frac{x_n + x_{n+1}}{2}, \frac{y_n + y_{n+1}}{2}\right)$ , and then you will have  $y_n$  or it will be  $y$  at  $x_n$  plus  $x_n$  plus 1 by 2. So, see we are looking at this uniform partition of interval  $a, b$ . So, you have got  $a$  this is  $x_n$  this is  $x_{n+1}$ .

The value here is  $y_n$  value here is  $y_{n+1}$  if you apply midpoint rule, then you are introducing one more value here. So, what we want is we want to determine approximation to  $y$  at the node points. We do not want to introduce some point in between and then those many values also coming into picture.

So, as such the midpoint rule directly it is not applicable now what one can do is instead of integrating between  $x_n$  to  $x_{n+1}$  you integrate from  $x_{n-1}$  to  $x_{n+1}$ . In that case, the midpoint will be  $x_n$  and that will give a rule, but that part we are going to look at it little later.

What will happen if I use trapezoidal rule? In case of trapezoidal rule, you consider the value at that two end points. Now what we are saying is, we have come up to  $y_n$  and you are going to determine  $y_{n+1}$ . So, if you apply trapezoidal rule your  $y_{n+1}$  will be determined only implicitly.

So, again that comes under predictor corrector formulae. So, that we will do little later now what I am going to do is , I want to consider interval  $x_n$  to  $x_{n+1}$  .I do not want to introduce new nodes like the midpoint of  $x_n$  to  $x_{n+1}$  and so on. I want to consider a cubic polynomial approximation .

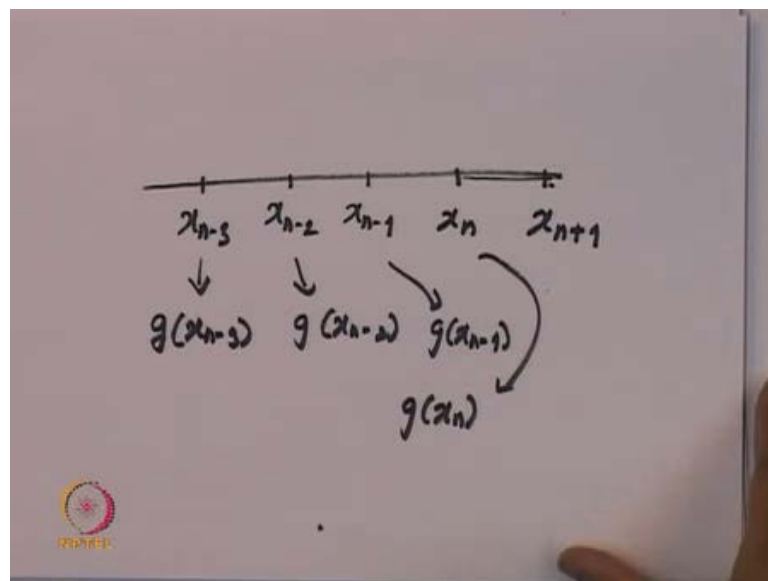
So, when you consider cubic polynomial approximation ,when we had considered Newton's cotes formulae ,what we did was we subdivided our interval  $a$  to  $b$  into we want to consider a four points; that means, three equal parts and then we fit a cubic polynomial I do not want to sub divide interval  $x_n$  to  $x_{n+1}$  into three equal parts because that will introduce new nodes. So, that I do not want to do.

But what I can do is I have come up to  $x_n$ . So, I know value at  $x_n$ , but I also know value at  $x_{n-1}$   $x_{n-2}$   $x_{n-3}$  . So, I can look at these four values fit a cubic polynomial and now integrate that cubic polynomial over the interval  $x_n$  to  $x_{n+1}$  .

So, this is something different to numerical quadrature we have done. So, far in the Newton cotes formulae, we would have sub divided we would have chosen four equidistant points in the in our interval of integration  $x_n$  to  $x_{n+1}$  .

So, there and then we would have fitted a polynomial ,now we are doing something else What we do is we go outside of our interval of integration. So, we

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have got we are integrating over  $x_n$  to  $x_{n+1}$ . So, you consider  $x_n$  minus 1  $x_n$  minus 2  $x_n$  minus 3. So, look at  $g$  of  $x_n$  minus 3  $g$  of  $x_n$  minus 2  $g$  of  $x_n$  minus 1 and  $g$  of  $x_n$ , fit a cubic polynomial based on these four points.

Once you get a cubical polynomial it is defined over whole of  $r$ . So, use its value over  $x_n$  to  $x_{n+1}$  and integrate because the cubic polynomial, you know how to integrate. So, that is going to give us a formula which is known as Adams Bashforth formula.

So, let me derive that formula. The computations they are straight forward, they are bit more complicated or if you want to really work out the details, now what I am going to do is I am going to consider the cubic polynomial interpolation, the points are equidistant. So, because the points are equidistant we can use our formula for cubic polynomial.

It becomes slightly simpler and we will try to put it in a form. So, that our integration becomes easier.

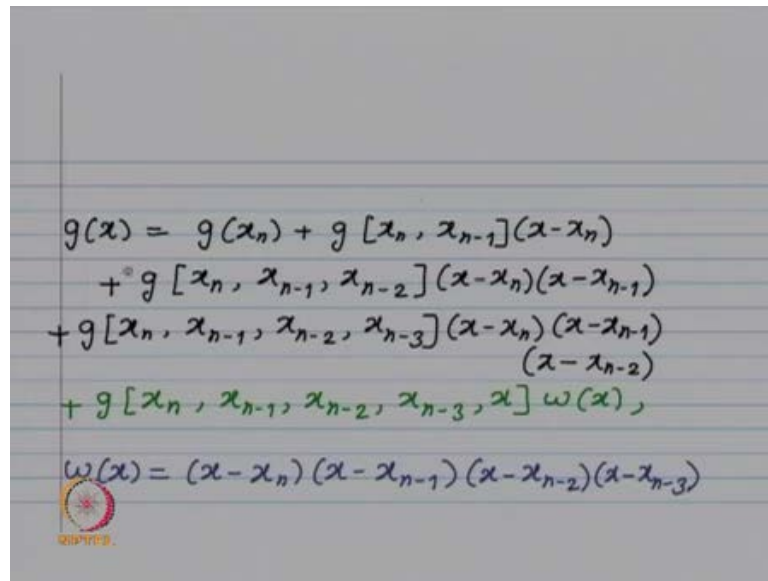
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$$y(x_{n+1}) - y(x_n) = \int_{x_n}^{x_{n+1}} g(x) dx$$

$p_3$  : polynomial of degree  $\leq 3$   
interpolating  $g$  at  
 $x_n, x_{n-1}, x_{n-2}, x_{n-3}$

So, we have got  $y$  at  $x_{n+1}$  minus  $y$  at  $x_n$  to be integral from  $x_n$  to  $x_{n+1}$  of  $g(x) dx$ .  $g$  is a function of  $x$ .  $p_3$  is a polynomial of degree less than or equal to 3 interpolating our function  $g$  at  $x_n, x_{n-1}, x_{n-2}, x_{n-3}$ . So, the interpolation points except for this  $x_n$  they are outside our interval  $x_n$  to  $x_{n+1}$ .

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The image shows a handwritten mathematical formula on a lined background. The formula represents the interpolation of a function  $g(x)$  using divided differences up to the third order, plus an error term. The error term is defined as  $\omega(x)$ , which is the product of  $(x - x_n)$ ,  $(x - x_{n-1})$ ,  $(x - x_{n-2})$ , and  $(x - x_{n-3})$ .

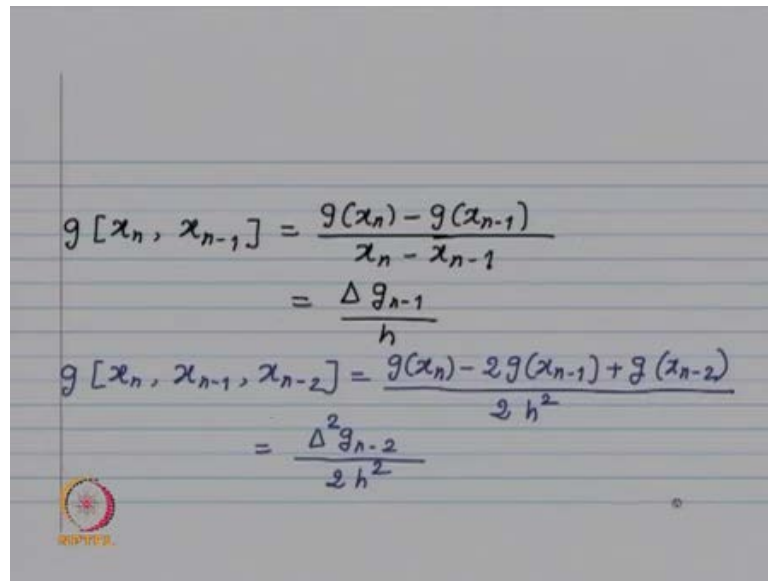
$$g(x) = g(x_n) + g[x_n, x_{n-1}](x - x_n) + g[x_n, x_{n-1}, x_{n-2}](x - x_n)(x - x_{n-1}) + g[x_n, x_{n-1}, x_{n-2}, x_{n-3}](x - x_n)(x - x_{n-1})(x - x_{n-2}) + g[x_n, x_{n-1}, x_{n-2}, x_{n-3}, x] \omega(x),$$
$$\omega(x) = (x - x_n)(x - x_{n-1})(x - x_{n-2})(x - x_{n-3})$$

Now, this is a formula you are familiar with  $g$  of  $x_n$ . So, this is the cubic polynomial  $g(x)$  plus divided difference based on  $x_n, x_{n-1}$  into  $x - x_n$  plus divided difference based on  $x_n, x_{n-1}, x_{n-2}$ .

Into  $x - x_n, x - x_{n-1}, x - x_{n-2}$  plus divided difference based on the 4 points  $x_n, x_{n-1}, x_{n-2}, x_{n-3}$  multiplied by  $x - x_n, x - x_{n-1}, x - x_{n-2}$ . So, this is the cubic polynomial and this is the error term.

So, in the error term, we have got  $x$  here and then  $\omega(x)$  where  $\omega(x)$  is product of  $x - x_n, x - x_{n-1}, x - x_{n-2}, x - x_{n-3}$ .

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The image shows handwritten mathematical formulas on a lined background. The first formula is  $f[x_n, x_{n-1}] = \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}} = \frac{\Delta f_{n-1}}{h}$ . The second formula is  $f[x_n, x_{n-1}, x_{n-2}] = \frac{f(x_n) - 2f(x_{n-1}) + f(x_{n-2}))}{2h^2} = \frac{\Delta^2 f_{n-2}}{2h^2}$ . A small logo is visible in the bottom left corner of the slide.

Next the divided difference based on  $x_n, x_{n-1}, x_{n-2}$ , will be  $f(x_n) - 2f(x_{n-1}) + f(x_{n-2})$  divided by  $x_n - x_{n-2}$ . This is  $2h$  and this is the Newton's forward difference  $\Delta^2 f_{n-2}$ .

So,  $\Delta^2 f_{n-2}$  is precisely  $f(x_n) - 2f(x_{n-1}) + f(x_{n-2})$  the divided difference of  $f$  based on these 3 points, you have got  $x_n - x_{n-2}$ , is equal to  $2h$ .  $x_{n-1} - x_{n-2}$  is also equal to  $h$ . So, this is equal to  $f(x_n) - 2f(x_{n-1}) + f(x_{n-2})$  and  $2h^2$  the quantity in the numerator is  $\Delta^2 f_{n-2}$ .

So, it is the Newton's forward difference of second order upon  $2h^2$  and now we will also write a similar formula for divided difference based on  $x_n, x_{n-1}, x_{n-2}, x_{n-3}$ .

That formula is

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$$\begin{aligned} &g[x_n, x_{n-1}, x_{n-2}, x_{n-3}] \\ &= \frac{g(x_n) - 3g(x_{n-1}) + 3g(x_{n-2}) - g(x_{n-3})}{6h^3} \\ &= \frac{\Delta^3 g_{n-3}}{6h^3} \end{aligned}$$

$g(x_n) - 3g(x_{n-1}) + 3g(x_{n-2}) - g(x_{n-3})$  divided by  $6h^3$ . So, upon  $6h^3$ . So, this will be the numerator is  $\Delta^3 g_{n-3}$  divided by  $6h^3$ . So, thus

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$$\begin{aligned} p_3(x) &= g_n + \Delta g_{n-1} \frac{x-x_n}{h} \\ &+ \Delta^2 g_{n-2} \frac{(x-x_n)(x-x_{n-1})}{2h^2} \\ &+ \Delta^3 g_{n-3} \frac{(x-x_n)(x-x_{n-1})(x-x_{n-2})}{6h^3} \end{aligned}$$

our polynomial  $p_3(x)$  is  $g_n + \Delta g_{n-1} \frac{x-x_n}{h}$  because the term here was divided difference based on  $x_n - x_{n-1}$  into  $x - x_n$ .

So, we have the divided difference to be  $\Delta g_{n-1}$  divided by  $h$ .



So, that h I am writing with  $x$  minus  $x_n$  the next term is  $\Delta^2 g_n$  minus 2 divided by  $2h^2$  into  $x$  minus  $x_n$  plus  $\Delta^3 g_n$  minus 3 divided by  $6h^3$  this is for the divided difference of  $g$  based on  $x_n$  minus 1  $x_n$  minus 2  $x_n$  minus 3 multiplied by this.

So, we have

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$$y(x_{n+1}) - y(x_n) = \int_{x_n}^{x_{n+1}} f(x, y(x)) dx$$

$$y_{n+1} - y_n = \int_{x_n}^{x_{n+1}} p_3(x) dx$$

Substitute  $s = \frac{x - x_n}{h}$

$$y_{n+1} - y_n = h \int_0^1 p_3(s) ds$$

got  $y_{n+1} - y_n$  is equal to integral  $x_n$  to  $x_{n+1}$  of  $f(x, y(x)) dx$ . This we are going to replace by  $y_{n+1} - y_n$  is equal to integral  $x_n$  to  $x_{n+1}$  of  $p_3(x) dx$ .

If I make change of variable here, as  $s$  is equal to  $(x - x_n)/h$  then I get  $y_{n+1} - y_n$  to be  $h$  times integral 0 to 1 of  $p_3(s) ds$ . So, we had our  $p_3(x)$  to be given by this. So, our  $(x - x_n)/h$  is going to be equal to  $s$  so  $x - x_n$  will be  $hs$  and so, on.

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$$y(x_{n+1}) - y(x_n) = \int_{x_n}^{x_{n+1}} f(x, y(x)) dx$$
$$y_{n+1} - y_n = \int_{x_n}^{x_{n+1}} p_3(x) dx$$

Substitute  $s = \frac{x - x_n}{h}$ .

$$y_{n+1} - y_n = h \int_0^1 p_3(s) ds$$

So, we have this h times integral 0 to 1 p 3 s d s

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$$p_3(x) = g_n + \Delta g_{n-1} \frac{x-x_n}{h} + \Delta^2 g_{n-2} \frac{(x-x_n)(x-x_{n-1})}{2h^2} + \Delta^3 g_{n-3} \frac{(x-x_n)(x-x_{n-1})(x-x_{n-2})}{6h^3}$$
$$p_3(s) = g_n + \Delta g_{n-1} s + \Delta^2 g_{n-2} \frac{s(s+1)}{2} + \Delta^3 g_{n-3} \frac{s(s+1)(s+2)}{6}$$

This is our p 3 x, x minus x n by h ,is x minus x n by h is s and x minus x n minus 1 by h is going to be equal to s plus 1, because we have

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$$\frac{x - x_{n-1}}{h} = \frac{x - x_n + x_n - x_{n-1}}{h} = s + \frac{h}{h} = s + 1$$

$x - x_{n-1}$  is equal to  $x - x_n + x_n - x_{n-1}$  divided by  $h$ .  $x - x_n$  by  $h$  is  $s$  plus  $h$  upon  $h$ . So, that is going to be equal to  $s + 1$ .

So, thus

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$$p_3(x) = g_n + \Delta g_{n-1} \frac{x - x_n}{h} + \Delta^2 g_{n-2} \frac{(x - x_n)(x - x_{n-1})}{2h^2} + \Delta^3 g_{n-3} \frac{(x - x_n)(x - x_{n-1})(x - x_{n-2})}{6h^3}$$

$$p_3(s) = g_n + \Delta g_{n-1} s + \Delta^2 g_{n-2} \frac{s(s+1)}{2} + \Delta^3 g_{n-3} \frac{s(s+1)(s+2)}{6}$$

we have  $p_3$  to be  $g_n$ , plus  $\Delta g_{n-1} s$ , plus  $\Delta^2 g_{n-2} s$  into  $s + 1$  by 2, plus  $\Delta^3 g_{n-3} s$  minus  $x_n$  by  $h$  will be  $s$   $x - x_{n-1}$  by  $h$  will be  $s + 1$ .

And  $x_{n+1} - x_n$  will be  $h$  times  $\int_0^1 \{g_n + \Delta g_{n-1} s + \frac{\Delta^2 g_{n-2}}{2} s(s+1) + \frac{\Delta^3 g_{n-3}}{6} s(s+1)(s+2)\} ds$ . So, distribute this  $h$  cube  $1$   $h^2$  each of the bracket and now

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$$\begin{aligned}
 y_{n+1} - y_n &= h \int_0^1 \left\{ g_n + \Delta g_{n-1} s \right. \\
 &\quad \left. + \frac{\Delta^2 g_{n-2}}{2} s(s+1) + \frac{\Delta^3 g_{n-3}}{6} s(s+1)(s+2) \right\} ds \\
 &= h \left\{ g_n + \frac{\Delta g_{n-1}}{2} + \frac{\Delta^2 g_{n-2}}{2} \left( \frac{1}{3} + \frac{1}{2} \right) \right. \\
 &\quad \left. + \frac{\Delta^3 g_{n-3}}{6} \left( \frac{1}{4} + 1 + 1 \right) \right\} \\
 &= h \left\{ g_n + \frac{\Delta g_{n-1}}{2} + \Delta^2 g_{n-2} \frac{5}{12} + \Delta^3 g_{n-3} \frac{9}{24} \right\}
 \end{aligned}$$

We have got  $y_{n+1} - y_n$  is equal to  $h$  integral  $0$  to  $1$  of  $\{g_n + \Delta g_{n-1} s + \frac{\Delta^2 g_{n-2}}{2} s(s+1) + \frac{\Delta^3 g_{n-3}}{6} s(s+1)(s+2)\} ds$ . So, you substitute and now you integrate. So, you will have first will be  $g_n$  then  $\Delta g_{n-1}$  integration of  $s$  will be  $s^2$  by  $2$  between  $0$  to  $1$ . So, that becomes  $\Delta g_{n-1}$  by  $2$  plus  $\Delta^2 g_{n-2}$  by  $2$ . Integration of  $s^2$  will be  $\frac{1}{3} s^3$  by  $3$  between  $0$  to  $1$ . So, it will be  $\frac{1}{3}$ .

Integration of  $s$  again  $s^2$  by  $2$ . So, it is  $\frac{1}{2}$  plus  $\Delta^2 g_{n-2}$  by  $6$  and now integration of this will be  $\frac{1}{4} s^4 + s^3 + s^2$ . When you simplify you will get it to be equal to  $h$  multiplied by  $g_n$  plus  $\Delta g_{n-1}$  by  $2$  plus  $\Delta^2 g_{n-2}$  multiplied by  $\frac{5}{12}$  plus  $\Delta^3 g_{n-3}$  multiplied by  $\frac{9}{24}$ .

$\Delta^2 g_{n-2}$  is  $g_{n-2} - 2g_{n-1} + g_n$  and the similar expression for  $\Delta^3 g_{n-3}$ . So, we substitute that

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$$\begin{aligned} y_{n+1} - y_n &= \\ h \left\{ g_n + \frac{\Delta g_{n-1}}{2} + \frac{\Delta^2 g_{n-2}}{12} + \frac{\Delta^3 g_{n-3}}{24} \right\} \\ &= h \left\{ g_n + \frac{g_n - g_{n-1}}{2} + \frac{5(g_n - 2g_{n-1} + g_{n-2})}{12} \right. \\ &\quad \left. + \frac{9(g_n - 3g_{n-1} + 3g_{n-2} - g_{n-3})}{24} \right\} \\ &= \frac{h}{24} \{ 55g_n - 59g_{n-1} + 37g_{n-2} - 9g_{n-3} \} \end{aligned}$$

and then we get it to be equal to after simplification you get the formula  $h$  by 24.  $455g_n - 59g_{n-1} + 37g_{n-2} - 9g_{n-3}$ . So,

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Adams - Bashforth Method

$$\begin{aligned} y_{n+1} &= y_n + \\ \frac{h}{24} [55g_n - 59g_{n-1} + 37g_{n-2} - 9g_{n-3}] \\ g_n &= g(x_n) = f(x_n, y_n) \\ y_0, y_1, y_2, y_3 &: \text{given} \end{aligned}$$

this is adams bashforth method.

Now, here when you look at the formula the coefficients, they are not very nice numbers, but it does not matter. You are going to write a program for calculating whatever are the coefficient that is once for all 1 does the derivation.

You write the program and then you know how to calculate the approximations to  $y_n$ . Now the formula which we obtain for  $y_{n+1}$  involves  $y_n$ ,  $y_{n-1}$ ,  $y_{n-2}$ ,  $y_{n-3}$ .

So, initially  $y_0$  is given to us. So, you cannot calculate  $y_1$ . So, you will be able to use this formula say  $y_5$  onwards. So, we have suppose  $y_0, y_1, y_2, y_3$  they are given to us, then using this formulae, you can calculate  $y_4$  or  $y_5$  onwards.

So, for  $y_4$  you will need  $y_0, y_1, y_2, y_3$  and then you can continue. So, that is why this method is not self starting, you have to somehow get  $y_0, y_1, y_2, y_3$  and then you can continue. In our next lecture we will see that here the discretization error is of the order of  $h^5$ , same as in case of Runge-Kutta method of order 4, but I will explain what I mean by essentially 1 function evaluation per step. So, we will do this and then in our next lecture, we are also going to look at what are known as predictor corrector formulae.

So, one of the methods which we are going to consider is known as Adams-Moulton method and then there are similar methods and we will compare these methods. So, thank you.