Numerical Methods and Simulation
Techniques for Scientists And Engineers
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Lecture 09
Numerical differentiation, Error analysis

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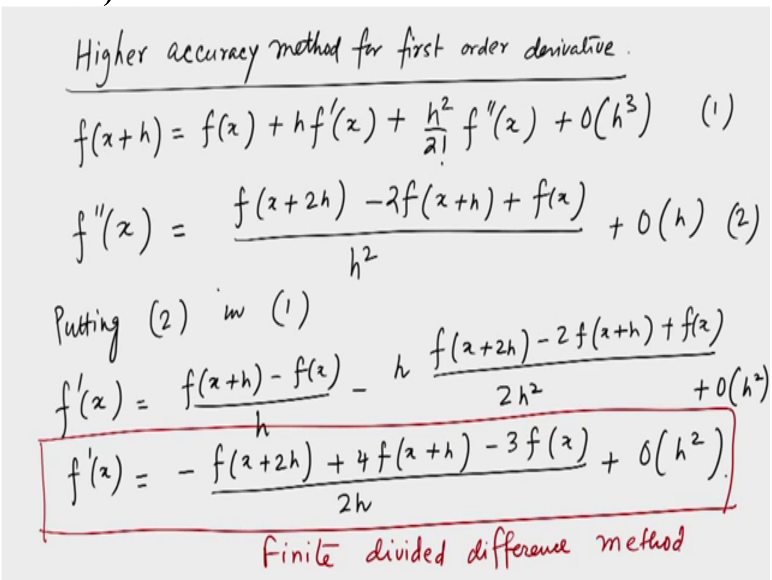

So, let us see one more technique of improving the accuracy of this first order derivative. So, this is so let us call it a higher order or higher accuracy method again for first order derivative. So, we will use the Taylor series that we have been using + a h f prime f x + h square by 2 factorial f double prime x and then what we neglect because of the truncation is h cube. So, just to remind you that we have of course we can ignore completely the double derivative and can arrive at a formula for the first derivative or the first order derivative that is f prime of x.

But here instead of that what we shall do is we will include the definition of the second order derivative and get an improved estimate or a more accurate estimate of the first order derivative. So, to remind you that the second order derivative is a second order derivative necessarily involves 3 points which could be you know f x - x x + 2h x of x + h and f of x or it could be f of x + h f of x and f of x - h it does not matter.

So, here we are writing it involving x + 2h the value of the function at x + 2h at x + h and at f of x that is at x so it is x + 2h - twice of x + h and a + f of x and this is nothing but divided by h square and we are leaving out terms which are of the order of h. So, we have used of course in the previous definition we might have used points such as f of x + h x and x - h here we have used 3 different points that is x + 2h and x + h and x but as I said that it does not make a difference.

So, if you put call this is 2 so if you put 2 in 1 that is I am going to put the second derivative into this third term that appears here and then do a slight bit of rearranging then we get as f x + h - f of x divided by h which is our original definition. And then there is a h and f of x + 2h - 2f of x + h - sorry this is + f of x so this is divided by 2h square because there is a factor 2 factorial which is nothing but 2.

And then if you realize that what we are leaving out is h square of the order of h square. So, if you rearrange or rather simplify this, this becomes equal to f of x + 2h + 4 f x + h - 3f of x divided by 2h and + of the order of h square and this so this is of the order of h square. So, this is a derivative formula for the derivative that you are one can use by you know explicitly using the definition of the second derivative.

So, this is another formula so instead of using the forward difference or the backward difference or the; you know the finite difference rather the; you know using a 3 point formula. We can also use this definition of the second derivative and put it into this into this equation or into this formula to compute the first derivative.

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Example $f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$

Find $f'(x)$ at $x = 0.5$ using finite divided difference method.

Use $h = 0.25$

Solution

$x - 2h = 0$ $\quad f(x-2h) = 1.2000$

$x - h = 0.25$ $\quad f(x-h) = 1.1035$

$x = 0.5$ $\quad f(x) = 0.9250$

$x + h = 0.75$ $\quad f(x+h) = 0.6363$

$x + 2h = 1$ $\quad f(x+2h) = 0.2000$

$$f'(0.5) = \frac{-0.2000 + 4(0.6363) - 3(0.9250)}{2(0.25)} = -0.8594$$

Exact Value $= -0.9125$

$$\text{Error} = \frac{-0.9125 - (-0.8594)}{-0.9125} \times 100\% = 5.82\%$$

So, let us see that how is it any better than what we know, so let us take an example all right so this is like f of x equal to - 0.1 x to the power 4 - 0.15 x cube - 0.5 x square - 0.25 x and a + 1.2 so that is the function that is given and find the first derivative that is f prime of x at x equal to 0.5 using this method and this method is called as a finite divided difference method. So, let us just write that so this is called as the finite divided difference method alright.

So, using this using a finite divided difference method that is the one that we have just learned which involves computing the or using the second derivative into the formula. So, I and it is given that I use h equal to 0.25 okay so the solution is as follows so you have x - 2h is equal to 0 because x is equal to 0.5 and 2h is equal to 0.5, so this is 0 so f x - 2h it is equal to simply 1.2 or I will write it with up to 4 decimal places because we use that.

This is just a arbitrary decision by us to use it for you know 4significant digits x - h is equal to 0.25 and f of x - h is equal to 1.1035 so if you put 0.25 into this then we can calculate this you know and it comes out as 1.1035 x equal to . 5 f of x is nothing but equal to 0. 9 2 5 0 and x + h which is nothing but 0.75 f of x + h is equal to it is equal to 0.6363 and finally the x + 2h which is equal to 1 so f of x + 2h is equal to 0.2000 okay.

So, these are the values that we are going to need and we can compute this using this method the method that we have just said and so on. So, f prime evaluated at .05 using that formula using this finite divided difference formula this is equal to – 0.2000 and 4 multiplied by .6363 – 3 0.9250 and divided by 2h so 2 into .25, so if you compute these correctly then it comes out as 0.8594 and the exact value of this exact value you can determine by because it is a 4 into 0.1 x cube and then put x equal to 0.5 and so on and then do this.

So, exact value is equal to you know 0.9125 and so error if you want to calculate this error so this is like minus which I should not forget so it is a -0.9125 and minus of -0.8594 divided by -0.9125 and if you want to convert it into percentage then it is this, this comes out as 5.82%, so using this finite divided difference method one gets an error of 5 nearly 6%t of error and one can actually test that with a lower accuracy method that finite-difference forward difference or backward difference or even the divided difference method what one gets.

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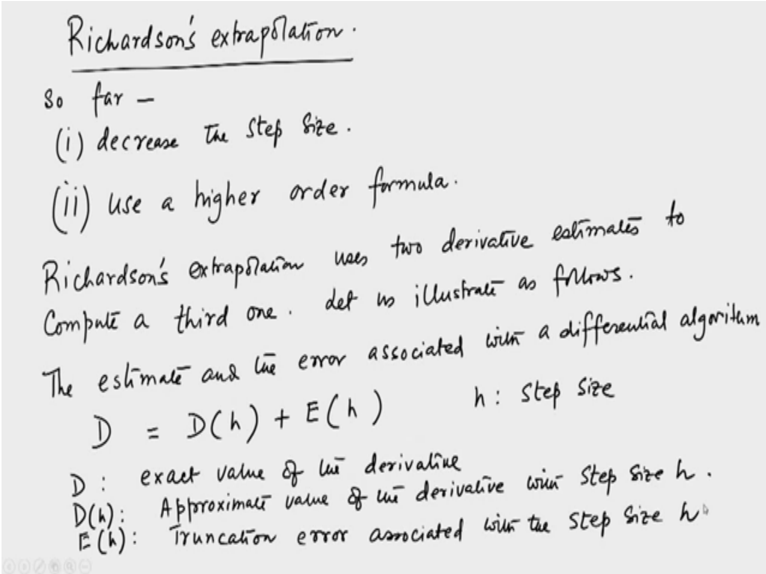

So, this is one example that we have, now let us learn about another method yet another method which is much more accurate and we will see that using the same example that you have seen here and that method is called as the Richardson's extrapolation okay. So, what is Richardson's extrapolation, so just to put things in perspective so far we have seen are 2 ways to improve the derivative of a function and one is that of course decreasing the step size this was not told explicitly.

But you should discover it yourself that if you have a step size of 0.1 you would get some result that is we talked about h the step size h and instead if you take a step size of .05 then you would get an improved accuracy because you are taking that the values of the function at really neighbouring points where you want to calculate the derivative. So, you are you know closing in the gap between the 2 points where you are computing the value of the function and both these points.

However this also comes with the risk of having if you have 2 less of a step size then the computer actually might you know get confused that to be 0 and there will be a division by 0 which is certainly not expected. But to a certain extent like in the last example we have taken a step size of 0.25 we could have reduced it to 0.1 and we would the 5.82%t of that error that we have obtained would certainly go down okay.

So this is one way of taking care of the accuracy of the derivative and the other thing is that we have which we have mostly used is that I use a higher order formula all right. So, if these are the 2 methods that we have seen so far what is this Richardson's extrapolation that is going to improve it? And we will see that it actually does a remarkable improvement of computing the first order derivative.

So, this Richardson's extrapolation uses 2 derivative estimates to compute a third one, so let us illustrate as follows okay. So, so basically the estimate and the error basically we are talking about the truncation error and the error that are associated with a differential algorithm is D that is the differential algorithm or the derivative that we are trying to compute it is D as a function of h which depends on the choice of h.

And hence the truncation error will also depend upon the choice of h and h needless to say is the step size which appears in the denominator of derivative. So, just to make our notations clear D is the exact value of the derivative. D h is the approximate value derivative with step size h and E h is basically nothing but the truncation error associated with the step size h.

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Now make 2 estimates using 2 step sizes, h_1 & h_2.

$$D(h_1) + E(h_1) = D(h_2) + E(h_2) \quad (\mathrm{I})$$

$f''(x)$ is independent of the step size.

Assume

$$\frac{E(h_1)}{E(h_2)} = \frac{h_1^2}{h_2^2} = \left(\frac{h_1}{h_2}\right)^2$$

: Importantly remove the second derivative from the problem.

$$E(h_1) = E(h_2)\left(\frac{h_1}{h_2}\right)^2 \quad (\mathrm{II})$$

Putting (II) in (I).

$$D(h_1) + E(h_2)\left(\frac{h_1}{h_2}\right)^2 = D(h_2) + E(h_2)$$

$$E(h_2) = \frac{D(h_1) - D(h_2)}{1 - \left(\frac{h_1}{h_2}\right)^2}.$$

So, if that is true then let us make 2 estimates using 2 step sizes namely h1 and h2. So, we will make 2 estimates of the same formula for 2 different step sizes h1 and h2. In principle h1 and h2 could be independent but we will see that we get a particularly simple formula if h1 and h2 have a relationship in between them. So, we will have the D h1 + E h 1 that is the error associated with h 1 or rather this is the exact value of the of the derivative for the choice of h 1 is same as D h2 + E h 2.

So, we choose the h 1 and h 2 such that basically the second so your second derivative. So, this can happen if your f double prime x which is the second derivative is independent of the shape step size okay. Because this double derivative will come into the expression of this Taylor expansion and if that becomes independent of the step size then we can write this for 2 different choices of h1 and h2 to be like this.

Assume or rather it is an assumption but at the same time this assumption we have seen said this h 1 and h 2 are related or they are you know only the truncation error is occurring only at the square of h, h 1 square and h 2 square refer to the discussion that we had last time over the truncation error. We are now assuming that it is not of the order of h rather it is of the order of h square. So, E of h 1 is nothing but proportional to h 1 square and E as for h 2 is proportional to h 2 square such that we can write down eliminating the constant of proportionality that the 2 errors are in the ratio h 1 square by h 2 square which is nothing but equal to h 1 over h 2 whole Square.

This importantly what happened does is they I mean what it does is that it importantly removes the second derivative from the problem okay. So, in any case we have to see this how it goes, so we have a E h 1 is nothing but E h 2 and h 1 by h 2 whole square so we are going to know reduce it to one variable that is E of h 2. So, we if we write it in this expression let us call this as you know one here we need to distinguish it from the 1that we have written earlier so we write it in Roman 1 and 2.

So, putting this a Roman 2 in 1 in 1 we have a D which is equal to or rather the D h 1 + now E h 1 I am going to replace it by this expression so this is E h 2 h 1 by h 2 whole square, so I am using 2 different step sizes and it is equal to D h 2 + E h 2 and if you compute or rather solve for E h 2 then it becomes equal to D h 1 - D h 2 divided by 1 - h 1 by h 2 whole square ok. So, that is the formula for E of or rather that is the error associated with this choice of h 2 which is you know the second choice for this step size.

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The truncation error is estimated in terms of the derivative and the step size. This (III) can be substituted into

$$D = D(h_2) + E(h_2).$$

$$= D(h_2) + \frac{D(h_1) - D(h_2)}{1 - \left(\frac{h_1}{h_2}\right)^2} = D(h_2) + \frac{D(h_2) - D(h_1)}{\left(\frac{h_1}{h_2}\right)^2 - 1}$$

In particular if one chooses, $h_2 = h_1/2$.

$$D = D(h_2) + \frac{1}{2^2 - 1}\left[D(h_2) - D(h_1)\right]$$

$$\boxed{D = \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1)}$$

Richardson's extrapolation formula.

So, what is it good at so now we have done the truncation error is estimated in terms of the derivatives and the step size and the step size okay. So, this can be substituted into this last one let us call this as 3, so equation 3 can be substituted into the parent formula. So, to say which is D h 2 + E h 2 so this is equal to a D h2 + D h 1 - D h 2 1 - h 1 by h 2 whole square or we can you know simply write it as D h 2 + D h 2 we can change the sign of both numerator and denominator and can write it like this.

So, this is the error associated with h 2 which are computed in terms of the values of the derivative at h 1 and h 2 where those derivatives can be either used using a forward difference formula or a backward difference formula or central difference formula. So, to say in particular if you choose h 2 equal to h 1 by 2 then one can have a D which is equal to D h 2 + 1 divided by 2 square - 1 D h 2 - D h 1 because this thing becomes you know a factor of 2 and so on.

So, this if you rearrange things and so on it comes out as 4/3 D of h 2 1 choice – 1/3 D h 1 the other choice so that is the formula that one can use in this Richardson's extrapolation. So, we call it as Richardson's extrapolation formula ok all right. So, this is the formula that we use for 2 different choices of h 1 and h 2 and then build up a third.

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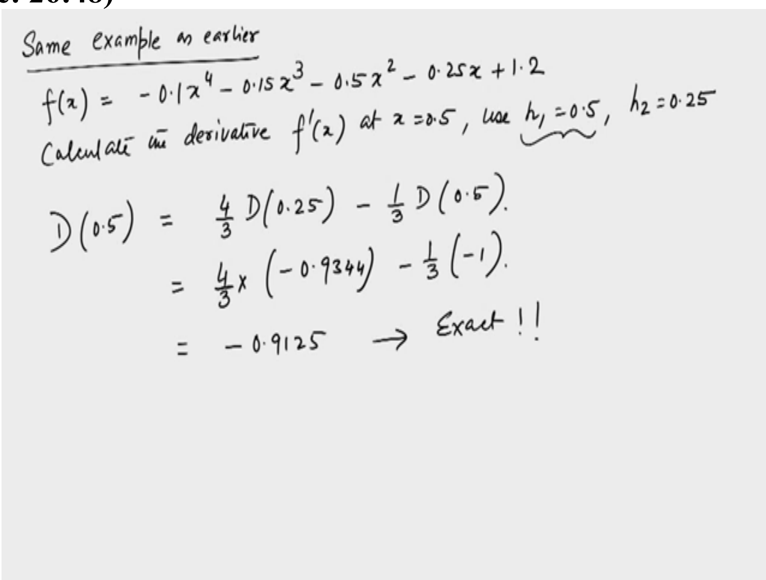

Let us see how this is more accurate or if at all it is so I will write down the example the same example once again. So, we have just to remind you so that you do not have to flip the pages or rather rewind the video. So, it is this - 0.5 I think we made a mistake it is so yeah that is fine .5 x square - 0.25 x + 1.2 and again calculate the derivative f prime of x at x equal to 0.5 in which case use h 1 equal to 0.5 h 2 equal to 0.25 because h 2 is nothing but h 1 by 5.

So, this is the thing that is given and h 2 we have automatically taken it to be the half of that h 1, so D at 0.5, that is you know h equal to 0.5 is nothing but 4 by 3 D equal to 0.25 - 1/3 D 0.5 ok. So, this is the thing now you have to calculate this D at 0.25 which you can use any of the methods we have used one particular method and this is like 4 by 3 in 2 - .9344 – 1/3 of - 1 and this is equal to - 0.9125.

So, this is absolutely exact that of course as you know as made us calculate these 2 derivatives at 0.25 and 0.5 using the best formula. So, we got the exact result using this Richardson's extrapolation ok. So, this is yet another improved method of calculating the derivative and of course in a particular case it gives you a result which is equal to you know exact result which otherwise you would have gotten if you do it analytically.

This was just coincidence that we have calculated this D at 0.25 and D at 0.5 for you know using formula which finally give you this okay. But it certainly is a better estimate of calculating the derivative. Now let us look at a practical issue of computing a derivative for unequally spaced point. So, sometimes when you are doing an experiment you may not be able to take data at regular intervals.

Or even if you do that there are some regions where the function is having an pathological behaviour that is the function is say blowing up or the function is having a kink or it is having a non monotonic behaviour you need to take much more data points there then at the places where the behaviour of the function is smoother. So, in those places where you need a derivative that is where the density of points are much more than at other places.

So, we can we can have a data set which are unequally spaced and for these unequally spaced data set we can use the Lagrange's interpolation polynomial that we have learnt earlier and analytically take the derivative, I will simply write down the formula and you can look at the Lagrange's polynomial that is interpolation polynomial and can convince yourself.

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Unequal spaced data points.

Lagrange's interpolation scheme using 3 points and analytically differentiating it at a particular point x_0.

$$f'(x_0) = f(x-h)\left[\frac{2x_0 - x - (x+h)}{[(x-h)-x][(x-h)-(x+h)]}\right] + f(x)\left[\frac{2x_0 - (x-h) - (x+h)}{[x-(x-h)][x-(x+h)]}\right] + f(x+h)\left[\frac{2x_0 - (x-h) - x}{[(x+h)-(x-h)][(x+h)-x]}\right]$$

So, we will use Lagrange's interpolation scheme and we are particularly taking it for 3 points using 3 points and analytically differentiating it for a particular point at or rather not for let us call it at a particular point say x 0 x 0 okay. So, what I mean to say is that the f prime at x 0 just like in the previous example the x 0 is nothing but 0.5. So, we will use this x - h and then this is that what we called as Li it is 2x 0 - x - x + h and this is x - h - x these are the data points.

So, these are like excise and these are x i - h so do not you know cancel x from here so this is a data point which is you know on the left of x differing by an amount h with a step size h and this is this the data point at x. And so this is like x - h and the - of x + h ok, this is these are the 2 data points and there is a value of the function at these left point. And + f of x and a 2 x 0 - x - h - x + h and then there is x - x - x - h and x - x + h these are analytically done from the Lagrange's interpolation polynomial.

You need to go back and check with the formula that we have written down there and similarly x + h is nothing but a 2 x 0 - x - h - and divided by x + h - x - h and x + h - x okay. So, this is the and it there is a formula for using the by using the Lagrange's undetermined or sorry Lagrange is interpolation scheme. It of course does not require you to have equally spaced data points you can have you know any 3 points of course here we have shown the 3 points as x - h and x + h and x.

But you in principle this works for any so we can have a x - h 1and x + h 2 and things like that and we can build the same formula for the derivative. So, this is for the use for the unequally spaced data points. As I said this particularly relevant when you have an inflection or if you have an upturn of a certain function non monotonic behaviour of certain function and that requires you to take much more data points in the vicinity of that inflection point or that upturn.

In which case if you need to find out a derivative there you need to use you know this is only used 3 points but you can use more points particularly in the context of an upturn or a non monotonic behaviour such as this. And so you may have a density of data points to be very, very large here whereas not so many data points once when the function becomes you know smooth like here you may not have those many data points and so on.

So, this is the main idea behind that so this is analytical you obtained and then you put it back into this into the computer to compute the value of the function say at a given point let us go x 0 I mean we are simply you know saying so this is your x and so on and this is your f of x I am just giving you a crude example of this. So, this by and large about derivative once again I reiterate that derivatives can become risky operation in computer because of these smallness of the denominator.

And sometimes the difference between quantities in the numerator can also be small. So, these small lesses are not really a good thing for a computer to compute. So, sometimes you know some derivatives are actually replaced or or other differential equations are replaced by integral equations where as integration is a much easier thing and a much more accurate thing to perform using a computer.

However nevertheless you still need to learn how derivatives are computed because at if you need to have a very direct answer to a question that where in the parameter space the function has a minimum or the function has a maximum one needs to calculate the derivative at all points in the vicinity of certain points which are hunched to have or which are suspected to have the housing the you know the minima or the maximum.