MATLAB Programming for Numerical Computation

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Module No. #03
Lecture No. #3.2
Numerical Differentiation – Differentiation in Single variable – 2

Hello and welcome to MATLAB programming for numerical computations. We are in module 3. In the first part of this module we are doing numerical differentiation in lecture 3.1. We considered how to compute f `(x) for a given function. In this particular module we are going to go forward and take 1 example which is of a practical nature as well as for a single variable problem find higher derivatives. Specifically, we are going to just look at f ``(x) for a couple of example problems.

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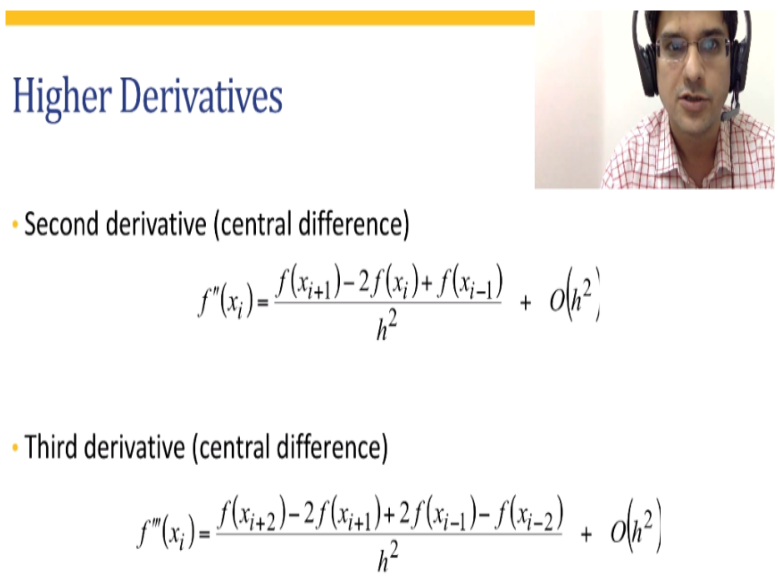

So, in previous lecture we have seen how to compute the first derivative. Now instead if we want to compute second derivative using central difference formula, we get f `` x is f(x+ h) - 2 f(x) + f(x- h) / h^2. Instead of writing (x+ h) and (x- h), I have given subscripts i+1, i and i- 1.

This central difference formula just as we had seen in the previous lecture is h ^ 2 accurate. We recall in the previous lecture f`(x) was given as f(x) i+ 1- f x i- 1 whole thing divided by 2h. That was the first difference, first derivative using the central difference formula. This is the formula for the second derivative; this is the formula for the third derivative and so on and so forth.

We can compute formulae for higher derivatives, over here this should be h cubed and not h Squared. In this lecture we are only going to concern our self with the second derivative over here.

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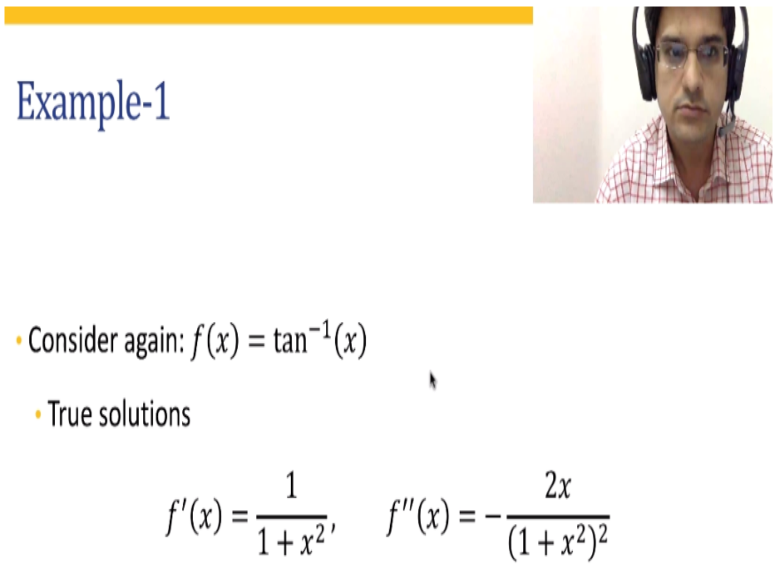

So, let us look at the problem again f(x) =to tan inverse of x and lets compute f ``(x). (Video Starts 02:08) Okay let us go on to MATLAB and we wanted to find f ``(x) at x = a and a is 1. Lets a h was 1 e- 4. (Video Ends: 02:25)

So, we wanted to compute f `` tan inverse f `` is given by this particular formula. (Video Starts 02:32) So trueVal = 2 multiplied by a divided by $1+a^2$, the whole squared a negative of that. And I will just put a negative sign. This is what our trueVal is. So trueVal is -0.5. (Video Ends: 02:53)

Let us compute the numerical derivative using the formula given over here. That is (a+ h) - 2f (a) + f (a- h) / h^2. f is nothing but a tan. (Video Starts 03:07) So, numDiff = atan (a+ h) - 2 times atan (a) - 2 * atan (a) + atan (a- h), a- h, let us put this all in brackets divided by h squared.

That’s going to be our numDiff. And numDiff is approximately equal to -0.5. The error between the difference between trueVal and numDiff is absval of sorry, abs (trueVal- numDiff). And the error is of the order of 1. 4* 10 ^ -8. (Video Ends 04:12)

So now that we have considered f ``(x) for tan inverse of x. Let us go on to the next example.
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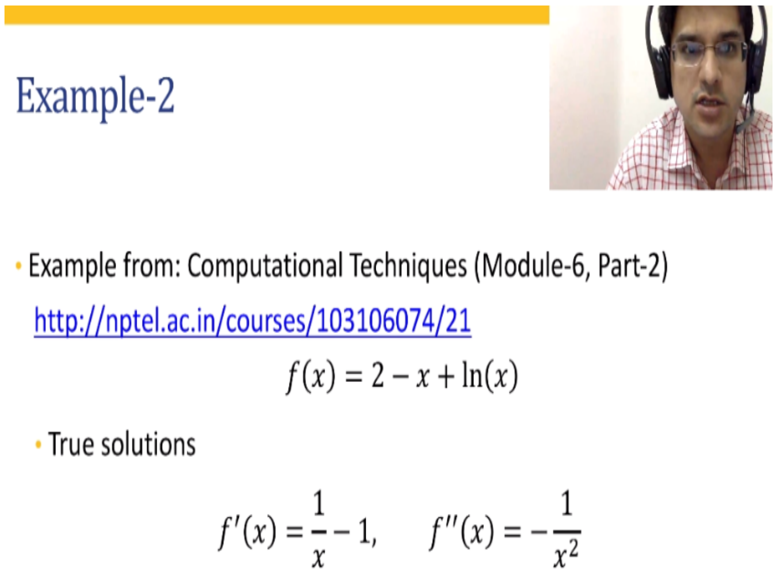

This example was taken from the computational techniques course module 6 part 2. For this f(x) is 2-(x+ ln x). What we are going to do today is, find f `x and f ``x for this particular function using central derivatives, I recommend what you may probably do at this stage, if you have not already tried to solve this particular problem from the previous lecture, is perhaps you can pause this lecture and take a few minutes in order to try solving f `x and f ``x for this particular example.

You might probably do it for just 1 value of step size h, let us say you take h = 10 ^ - 4 and try to solve this problem. Meanwhile I will give you a solution for this problem in MATLAB as well. (Video Starts 05:22). Okay, I have cleared the screen. Let us say edit numDiff2, numerical differentiation for the second problem 2- (x+ ln x).
Let us say we wanted to find this at, let us perhaps say that we want wanted to compute this again. At x, a = 1 and h = 1 e- 4. Let us say we call f(x+ h) as f1, f(x) = f2 and f(x- h) = f3. So

that is going to be 2-a. Sorry, 2- (a+ h) in fact I write at this way x = a+ h, f1 = 2- (x+ log(x)). And we copy paste. x = a and f2 = this, x = a- h and f3 = this.

TrueVal, trueVal 1 let us called as for f ` and that is going to be 1 /(x- 1). So 1 / (a- 1). trueVal2 is – 1/ a^2. So this is what we need for numerical derivatives. numDiff1 is nothing but. (Video Ends 04:12)

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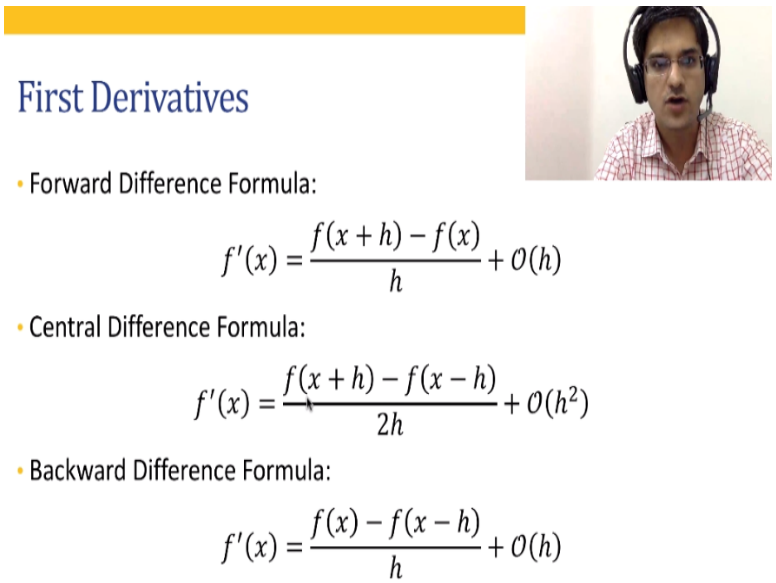

Yeah so f` x was f1- f3 divided by 2h. (Video Starts 07:55) f1- f3 divided by 2 multiplied by h. numDiff2 was f1- 2f2+ f3, f1- 2 multiplied by f2+ f3 divided by h squared. That is our numDiff2. err1 = abs (trueVal1- numDiff1). Actually, rather than saying numDiff, we will call this as numVal.

Press shift and enter. So all the values will get changed and the numVal2. So that is err1 and err2 = abs (trueVal1- sorry trueVal2- numVal2).Let save this and run this. So we will get err1 is 3 *10 ^- 9, err2 is 5 * 10 ^ 9. If we check numVal1 that is 3*10 ^- 9, when we expect trueVal1 as 0, numVal2 is- 1.

We are expecting trueVal also to be sorry, trueVal2 also to be equal to - 1. So as we can see that the errors using central difference formula are for h = 10 ^ - 4 are very small. (Video ends 10:05)

So now that we have completed the numerical differentiation for the second example 2-(x + ln x).Let us now head on over and look at a practical problem of a practical interest.

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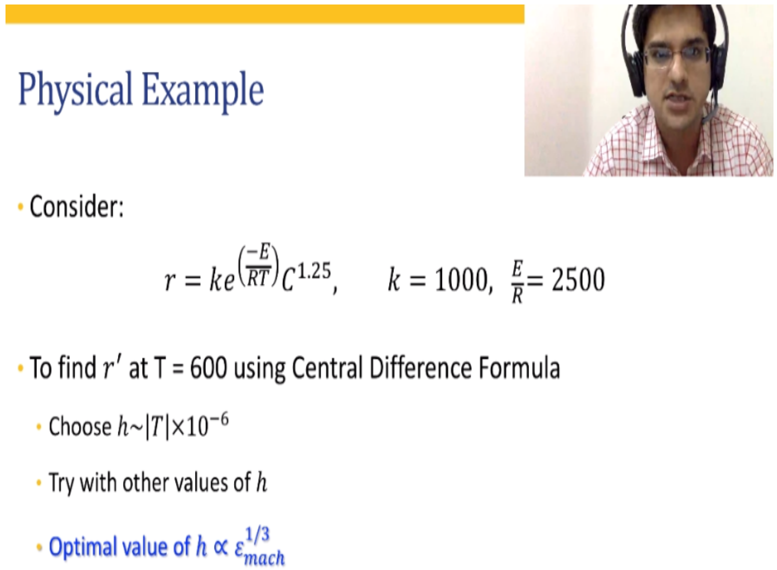

This comes from chemistry. As you all know that the rate of reaction can be return in the Arrhenius form given over here. So, rate r is k multiplied by e ^ - e / rt multiplied by the concentration to the power 1.25. The rate constant k= 1000 and e/r = 2500. Let us go on MATLAB and try to solve this problem.

(Video starts 10:46) And edit reaction rate differentiation r = k multiplied by e ^ - e / rt * c ^ 1.25. Constants a equal to and e by r equal to, so, k was 1000 and e / r is 2500. Differentiation do this at c = 1. 0 and t = 600 right. Okay, so now the analytical derivative for this guy. So temperature is the thing that is vary so because its - e ^ e / rt it is basically going to be e / r t squared okay multiplied by the rate r itself.

So, let us first calculate the rate r = k * exp - e/ r / t, multiplied by c ^ 1.25. That is the rate, trueVal is just going to be equal to r multiplied by e / r / t^2. That is our trueVal. Now then for the numerical differentiation we want to calculate r1 and r1 is going to be nothing but k multiplied by e to the power this guy. But instead of t we will have (t+ h). So let us just copy this. And we will put (t+ h) over here using central difference formula. Let us copy and paste this over here. And r2 is going to be this but it is going to be (t- h).

And numVal is going to be equal to nothing but r2- sorry, r1- r2 / 2 * h. Now the question is what is the value of h that we need to take. So, h that is just take that as we had been doing this before let us just take h = 1 * 10 ^- 4. And error is going to be equal to abs (trueVal- numVal).

Let us save and run this problem and we hope that there is no error and this runs and the error, that is the difference between the trueVal and numVal is 4 * 10 ^ -11. The trueVal is 0. 1077 and numVal will also look same 0. 1077. (Video ends 14:32)

So, that completes our exercise of finding dr / dt at t = 600 kelvins using the central difference formula. Where, the r is the rate of chemical reaction of the Arrhenius form. What you can try to do is, see the effect of other values of h how increasing or decreasing the value of h changes the errors in dr / dt.

We had seen in the previous lecture is that the optimal value of h is machine precision to the power 1/3 for central difference formula for f `(x). The machine precision to the power 1/3 is when the overall temperature or x, the independent variable is of the order 1. If the independent variable is of a different order, the optimal value of h changes accordingly, prior to look at this example.

We look at the other example 2- (x+ ln x) and computed f `(x) as well as f ``(x) for central difference formula of f`(x). The optimum value of h happens to be epsilon ^ 1 /3. Whereas, for the second derivative central difference formula the optimal value of h is epsilon ^ 1/ 4. This is also something that you can probably verify as a practice problem.
In the next lecture, we are going to revisit this physical example of this rate of reaction. With this I come to the end of lecture 3. 2 and I will see you in the next lecture. Thank you and good bye.