

MATLAB Programming for Numerical Computation
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Module No. # 03
Lecture No. #3.1
Numerical Differentiation – Differentiation in Single variable

Hello and welcome to MATLAB programming for numerical computations. We are in module 3 and in this module we are considering numerical differentiation and numerical integration. In the first 3 lectures of this module, we will go over numerical differentiation and then in the final 3 lectures of this module we will go over numerical integration.

This is lecture 3.1. In this lecture, we are going to cover differentiation in single variable. Primarily this lecture is going to focus on first differences that is $f'(x)$ given $f(x)$. In module 2, we had covered forward difference formula for $f(x)$. So the forward difference for $f(x)$ is given over here. $f'(x)$ is given by $f(x+h) - f(x)$ the whole thing divided by h . We saw that this method was order h^1 accurate. That was the forward difference formula.

(Refer Slide Time: 01:13)

First Derivatives

- Forward Difference Formula:

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)$$

- Central Difference Formula:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2)$$

- Backward Difference Formula:

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \mathcal{O}(h)$$



The other formulae for first derivatives are given over here. The forward difference formula as we just said was $f(x+h) - f(x)$ the whole thing divided by h the accuracy is h^1 . Central difference formula is more accurate than the forward difference formula. And the central

difference formula is $f(x + h) - f(x - h)$ divided by $2h$. What that means is, if you want to find a derivative at $f(x)$, we take a 1 point before that particular 1 point, after that particular point and find a slope using those 2 points. That is what a central difference formula is.

You probably already know from your mathematics course, that central difference formula is more accurate than the forward difference formula. It is h^2 accurate. What that means is every time we decrease the h by a factor of 10, the error also decreases by a factor of 100, not factor of 10. Why that is so, that is because it is h^2 accurate and the backward difference formula is given over here.

(Refer Slide Time: 02:25)

Example

$$\begin{array}{lcl} \frac{\tan^{-1}(1+10^{-4}) - \tan^{-1}(1)}{10^{-4}} & \varepsilon=5e-5 \\ \left[\frac{d}{dx} \tan^{-1}(x) \right]_{x=1} & \frac{\tan^{-1}(1+10^{-4}) - \tan^{-1}(1-10^{-4})}{2 \times 10^{-4}} & \varepsilon=2e-9 \\ \frac{\tan^{-1}(1) - \tan^{-1}(1-10^{-4})}{10^{-4}} & \varepsilon=5e-5 \end{array}$$

What we are going to do is, we will take the same example that we covered in module 2. That is tan inverse of x and we will find out the forward, central and backward difference formulae for that particular problem. We will do that for $h = 10^{-4}$. So let us go to MATLAB and do this problem.

(Video Starts 02:46) So, edit numDiff1 okay. Comparing numerical differentiation formulae for $f(x) = \tan^{-1}(x)$ at $x = 1$ okay. So $a = 1$ and trueVal is going to be equal to $1/\sqrt{1+a^2}$. And our h is 1.0×10^{-4} okay. The forward difference formula.

Okay, forward difference formula is $\tan^{-1}(a+h) - \tan^{-1}(a)$ divided by h okay. FwdDiff equal to $(\tan(a+h) - \tan(a))$ divided by h okay. And we need to put brackets over here because the entire numerator needs to be divided by h . Error in forward difference formula is $\text{abs}(\text{trueVal} - \text{fwdDiff})$ okay. Central difference ctrDiff equal to let us go over here, $(\tan(a+h) - \tan(a-h))$ divided by $2h$ okay.

So $(\tan(a+h) - \tan(a-h))$ okay. This needs to again go in brackets we remember divided by h sorry, divided by 2 multiply by h . And again the denominator also goes in brackets, errCtr, remember these brackets in both the numerator as well as the denominator okay.

Error in central difference formula is $\text{abs}(\text{trueVal} - \text{ctrDiff})$ okay and we will just copy and paste this for backward difference formula. Backward difference formula bkdDiff is, bkdDiff is $(\tan(a) - \tan(a-h))$ divided by h . So let us make that change. So $(\tan(a) - \tan(a-h))$ divided by h . errBkd, bkd is absolute value of $\text{trueVal} - \text{bkdDiff}$ okay. So let us save this and let us run this and see the results okay. So we have run this and we now have the results over here.

The error in backward difference formula is 2.5×10^{-5} . Central difference formula is 8×10^{-10} , the forward difference formula is also 2.5×10^{-5} . If we want we can go over here and we can display the results using disp. As we had seen earlier, disp error in forward difference is num2str, errFwd close this and this will display the error.

And likewise disp error in central difference is num2str, errFwd. Let me not change this errFwd and just run it and see what actually happens okay. You know what to expect over here. I just want to show that because this is actually a very common error. I mean come to think of it, you will think that these are small things that we will not make an error.

But these are again small things, its human exercise, writing a code is a human exercise and these things are ought to happen. So, I am just showing you some of the common things that the end of doing. In fact, I myself do this type of errors a few times and these errors sometimes are fairly difficult to detect. So let me run this and see what happens ok.

So, what happens when I run this is error in forward difference formula is, 2.5×10^{-5} and error in central difference formula again is 2.5×10^{-5} . So this should raise a suspicion. So, why are you getting the same results and we know why we are getting the same results because, not because we made a mistake in calculating the central difference formula. We forgot to change this errFwd to errCtr okay.

So, we just do that save and run this. And now we will get the correct results. Error in forward difference is 2.5×10^{-5} and error in central difference is 8.3×10^{-10} . So we see that the central difference formula is much more accurate than the forward difference and the backward difference formula okay. So, we finished this particular example. (Video Ends 09:22)

(Refer Slide Time: 09:26)

The Choice of h in Differentiation



- Order of accuracy:
 - Previous example was done for $h = 10^{-4}$
 - Repeat for a range of values, $h = \{10^{-1}, 10^{-2}, \dots, 10^{-5}\}$
 - Make a log-log plot
- Recall Module 2: Tradeoff between Truncation and Roundoff Errors
 - Repeat for a range of values, $h = \{10^{-1}, 10^{-2}, \dots, 10^{-10}\}$

So what we have seen is, we have done this particular example for 10^{-4} . What we want to do now is, repeat for a range of values. Recall that we are done this in module 2 using a for loop. Now we are going to do this not using a for loop but using array operations.

(Video Starts 09:49) Ok and let us go over here. What I will do is, I will comment out all of this so that we only focus ourselves on forward difference formula. You right click and click on comment. Once you do that the entire thing will become be commented out and this will not run. I will delete this display also. Because we do not need okay.

So, now what we want to do is, we want to do this for $h = 10^{-1}, 10^{-2}, 10^{-3}, -4$ and -5 okay. We can do this using array operation. So instead of giving h as a single value, we can give h as an array 10^{-1} in steps of -1 up to -5 okay. So this guy is going to give us a vector which is $-1, -2, -3, -4, -5$.

We are going an element by element power. This is important, we are doing an element by element power a of 10 . So which will lead to our h be equal to 10^{-1} to $2, 3, 4$ and 5 ? Let us highlight this and evaluate this right click evaluate selection and see what we get indeed we get h equal to $10^{-1}, -2, -3, -4, -5$ okay.

Let us go over here and look at what happens. When we give this numerator, let me highlight just the numerator. Right click along with parenthesis, let me highlight it right click and click on evaluate selection okay. Now we have not defined our a , so $a = 1$ sorry about that okay. And let us reevaluate this particular guy and press enter okay. We again get a vector okay. $\tan(a+h) - a$. $\tan(a)$ is a vector.

So, now what we are doing is we have a $1/5$ vector in the numerator and we have a $1/5$ vector in the denominator. And we are dividing it okay. There is another problem over here. We need to make another change okay. I will not tell what the change to be made is. Can you spot what other change need to be made? Okay.

I will pause; you can pause this video and think about what is one more change that we need to be made in order to compute the forward difference formula over here. I will run this code and let us see what actually happens. What we are expecting is forward difference formula to be a $1/5$ vector. Let us see what we get. FwdDiff, forward diff is not a $1/5$ vector but instead is just a single value okay.

And the reason for this is by doing this slash we are not taking an element by element division. But actually we are doing what is known as least squares. Do not worry about what we are actually doing over here. This is something that we will probably cover in module 6 of this course okay.

You should not be using slash for element by element division. But you should be using dot slash because we want to do an element by element division. Let us save this and run this and see what results we get okay. Let us plot on a loglog plot h verses errFwd . And we will get this straight line.

Remember this is the result that we had already obtained in module 2. We had done that using a for loop. Now we have resolved it using array operations in MATLAB okay. (Video Ends 13:58)

So let us now look at this for a range of values of h from 10^{-1} to let us say 10^{-12} okay. (Video Starts 14:11) But before that we will also do this for central and backward difference formula. So let me highlight this. Right click and click on uncomment okay. Remember all the thing that we needed to change is be needed to convert our h into a vector.

And the only thing that we needed to change over here was a dot slash, nothing else was required and that is because a \tan itself takes when it is gets a vector. It will give a vector as a result where tangent values obtained it for an each element and $2 * h$. We do not need a dot star because this is a scalar multiplication. So none of the other things are changed and let us do this.

Let us plot the results. We need to plot at on a loglog plot h . fw sorry, errFwd , blue line h , errCtr . Let us say a-redline and h errBkd as a . - magenta line okay. Save and run this and see what results we are getting okay. The magenta line and the blue line lie almost on top of each other okay. And the errors in forward and backward difference formulas are greater than the error that we see in central difference formula okay.

Now let us increase this to, let us say 10^{-10} and see what we get okay. If you recall what we have done in module 2, what we should be getting is, we will be getting minima in error at certain value of h . The value of h is going to be different for forward difference formula and for central difference formula. That is what we will see. So let us clear all okay.

Let us save this and let us run okay. So what we get is, that the error in forward and central, backward difference formula. All error in central difference formula also falls. And there is a minimal. The minima for forward difference and backward difference formula happen at 10^{-8} . Whereas the minima for central difference formula happen at 10^{-5} okay.

The actual place where the minima happen is $\epsilon^{1/2}$ for forward and central forward and backward difference formula and at $1/3$ for central difference formula. So the minimum in the error is at 10^{-8} for forward difference formula. And approximately around 10^{-5} or 10^{-6} for the central difference formula okay. (Video Ends 17:16)

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The Choice of h in Differentiation



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 - Make a log-log plot
- Recall Module 2: Tradeoff between Truncation and Roundoff Errors
 - Repeat for a range of values, $h = \{10^{-1}, 10^{-2}, \dots, 10^{-10}\}$

Let us see what we have. So recall module 2, tradeoff between truncation and round off error. We see similar tradeoffs in forward and central difference formula also okay.

(Refer Slide Time: 17:29)

Example-2 (for Practice)



- Example from: Computational Techniques (Module-6, Part-2)

<http://nptel.ac.in/courses/103106074/21>

$$f(x) = 2 - x + \ln(x)$$

- True solutions

$$f'(x) = \frac{1}{x} - 1$$

So this the theoretical ideas behind this were covered in computational techniques course module 6 part 2 the link for which is given over here. So if you are interested in getting a theoretical understanding of why we get minima at a various values for forward and central and backward difference formula, you can go to this video lectures and view those video lectures okay.

In that lecture, what we have done is, we have taken $f(x) = 2 - x + \ln x$ and computed forward, central and backward difference formula for that particular problem. And the true solution is given by $1/x - 1$ okay. So this is a problem that we may want to solve for practice okay. So with that I come to the end of lecture 3.1. In this lecture, we have covered forward, backward and central difference formula for calculating $f'(x)$. Thank you and see you in the next lecture.