Scientific Computing Using Python

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Lecture No. 07

Welcome to Scientific Compute Using Python. So today we begin our main course: Scientific Computing. Today, in the lecture, we will discuss how the errors in our computation evolve. How do we discuss it? How do we affect our computation? So, let us discuss it today. So, let us start.

Today's lecture will be basically on errors in computation. Whatever work we do in Scientific Computing, we are going to take help of the computer. We are going to do programming with Python. So, what will happen in it is that some error occurs. So, what are the errors? We will discuss that.

Now look, there is a computer. In the computer, if I write 2, if I define 2+3, then 5 will come as the answer, and this is our 5 answer. And the problem arises in the computer that if I write pi, then what will it do?

Now, pi is an irrational number, and the irrational numbers are non-terminating and non-reckoning. But if we use pi in our computation, then it will truncate the pi somewhere, or it will truncate it to 10 digits or 16 digits. If I want to write a 1/3 in a computer, then what will it do? 0.333 will keep going. It is a repeating number or a rational number. So, what will it do in this case? It will truncate this number somewhere or it will do an evaluation of error. It will generate a truncation error or roundoff error. It usually happen when dealing with rational numbers or irrational numbers.

So, that is why we study it. There is a name for it: floating point representation. So, we define what is the meaning of floating point representation.

So, what happens in it? Floating point means it is coming to us in the form of decimal. So, we have defined it. The number that we have is like this: .d1d2d3, like dk into some 10 to the power. If I am taking it in decimal form, then 10 to the power some e. So, we can use it in decimal form; we can use it in binary form. So, in binary, instead of ten, two will come.

If we define a decimal form like this, then we call the decimal form — this part is called mantissa, and this part is called exponent. 1/3, we can take it like this, right? In the 1/3 that we got, 1/3 will go on like this: 0.3333. The value of pi is 3.14 something, so that will go on. So, all these will come under the category of floating points.

Okay, what is di’s here? These are integers, decimal values. Between one and nine, they can take any value. They will not take d1zero, but otherwise, it can be any value from zero to nine. Okay, so we can write it as: where each di is between zero to ten. And exponent we know that the values can be positive as well as negative.

So now, how can we take the representation of the number, is our main question. Because if we have any values , we have values suppose I write 1.234×10^2. I write this, so what does it mean? This is equal to 123.4. So, I can write it like this also. Why can't I write it? I can write it like this: 12.34×10. Right?

So, we can write it in any form. I multiplied it by 100, so we got two decimals. Okay, so this value came. I just multiplied it by 10 and put 10 here, so we got 12.34×10. So now, what are we doing? That how do we define whatever floating points are there in a standard way? So, we have to discuss that.

The first thing is how to represent any number in a standard way. How can we say that this value will be considered as a standard value? So, what do we do for that? We give a name to the floating points. We define them in a form, and we call that form normalized form.

So, what is normalized form? Normalized form is that we have any number. We take any number. We represent it as x. The values that are p multiply 10 to the power of q are represented in this form. So, what did we do? We defined a number in this form, and we wrote that if our value is positive, there is no problem if that negative value. If it lies between point one to one. And q will be an integer only. So, we will say that these values are normalized.

This is the normalized form. Any value, like I had done this — so in this, neither this is the normalized value, nor this is a normalized value, this is also not a normalized value. Okay, so if I want to write this in normalized form, then what will I do? I will write this as 0.1234 into 10 to the power 3. We do this, now that we have p, so this is my suppose x. So, our p is here. What is the value of p? p is 0.12 and it lies in this range. So, we can say that this is the normalized form of our number. So, let's fix this that we have to write it in normalized form. There is another form of the number, we call it scientific.

So, what is in scientific form? If the value of p, which we have, if it is between 1 to 10, then we will say that it is a scientific value or scientific form. So, this is our scientific form. Why? Because the value of p is 1.2 which lies between 1 and 10 ,then it will come in scientific form.

So, what will we do? First of all, if we get any number, we will try to write it in normalized form. So, we will normalize it because we need a standard that how can we take a number.

Now, for example, this is a number, we call it floating point because its representation keeps floating. For example, this is a number — I can write it like this, then I also wrote it as..., then I also wrote it like this. So, we are writing the same number in different ways. So, we call it floating point.

Now, I have 5. So, for example, if we define the integer value 5, then we will write it like this. But the problem arises when we deal with fractions. So, if we have to deal with fractions, then what will we have to do? We will have to give it a form — what standard form should we keep, so that any number should be kept in that standard form only then we can use it.

So, what did we do with it? We have defined it in normalized form, that we will keep it, we will keep it in normalized form. Right? So, this is the work that we do. Now, let us see how the error evolves.

Now, for example, the first error that occurs is called round-off error. Now, round-off error you guys know that if we have values, let me take the value of pi. Right?

So, we have used pi the most. So, how have we been calculating the value of pi since childhood? We calculate it in approximations that is 22/7. Right? But we know that pi is an irrational number, and 22/7 is rational, but still we use it. Why do we do it? Because its value is the same up to a few digits.

Now, for example, if we see, if I write 22 by 7, it is rational. Then its value is 3.142857. It comes. After that, it will repeat: 142857, 142857 — so these values are repeating. Because rational numbers can be non-terminating as well, but they will be repeating or they will get terminated, like 1/2. So, 0.5 is terminated. Okay? It is a rational number. This is also a rational number, but it is non-terminating, it will never terminate but will keep on repeating.

So, what do we do with this? We cannot write pi as approximations from this, we can write pi as 3.14. But if we have to do high computation, then what do we do? That we do computation up to high digits. Like if we have to do scientific computing, we have to launch satellites or launch something and see what will happen 50 years or 20 years or 30 years from today, so what do we do in that?

The computation that happens is done up to 50 digits to 100 digits. So, in that case, the error that we have, it happens because the error in it has evolved.

How has the error evolved? The value of pi is something else, but we wrote it as 3 and used it. So, what did we do? The error that we have got evolved. So, if we calculate this error further, then this error can increase. Right?

So, if it keeps on increasing, then we came to know that in the beginning we thought that the error is very less, but going forward the error increased a lot. So, we will see how to deal with this work. Okay, so what did we do? That is, how to look at this error. So, we start with rounding off error.

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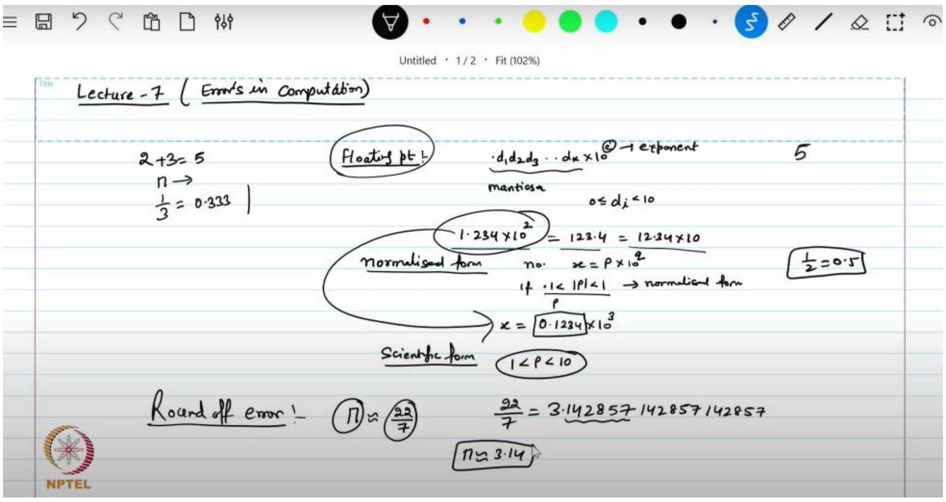

So, what is rounding off error? We know that if we go somewhere, to a shop, then suppose at the shop you get a bill of ₹20.45 paisa. So, what do you do? You know that the 45 paisa that you have is not available. It is not there at all. Even the shopkeeper says to you that okay, you give me ₹20. So, what did we do? We rounded off the amount and took out 20 values.

What happens sometimes is that you go to shopkeeper, and suppose the bill that comes to you is ₹20.75 paisa. So, what happens in this case is that the shopkeeper will say to you that you give me ₹21. So, what did we do? The shops are well defined. So, there are different shops like yours. There is a Safal shop, there is Mother Dairy. So, what did they automatically do? That if your values are less than 50 paisa, then you will give the lowest value. ₹20.45 which was our amount, we will give ₹20. And if these values are more than 50 paisa on this side, then we will give extra value.

So, what did we do? Whatever are the 20 point something values here. So, this can either become ₹20 or it can become ₹21 depending upon what these values are. So, if this value is less than 50 paisa, then you will have to pay ₹20. And if it is greater than 50 paisa, then you will have to pay ₹21. So, we have defined this.

Now the question arises that what will happen if it is exactly 50 paisa? So, if 50 paisa is exactly, then if we have 50 paisa available, because we have a 50 paisa coin, we will provide that and give it to them. So, if we get a bill of ₹20.50, then we will pay the full amount. The problem is how to pass below that and how to pass above that. Even if it is ₹20.50, then also we can say that let's pay 20. It depends on what the shopkeeper charges you. He charges ₹20 of ₹21.

So, there is a rounding off error. Rounding has always been done. So, how to do the rounding off mathematically, we have to see. So, now what do we do in rounding off? There are two ways in which we do rounding. So, we write round. Now let's see what is there in it.

So, one is chopping. Or instead of writing rounding, we say that it is a number. How can we terminate it? So, instead of writing it like this, we write this. How can we terminate the number? So, one way is chopping and another is rounding. So, we have to do rounding and we have to do chopping. So, you see how to do it.

Now, so we have a number. This is 0.1686 into 10 to the power 3. I took such a number which is in normalized form. So, what did we do? We chopped it. Now we have to do chopping. How to do it? Suppose I am doing chopping after three digits. So, after its three digits, I have to do rounding as well and chopping as well. So, what will be the three digits? Its first is this, second is this, third is this, fourth is this. We have to do chopping.

So, in chopping we will directly chop it and its value will come out to be 0.168 into 10 power 3. We do not have to see what the next number is. We just do chopping. What we will do in rounding is we will see its value and if its value is greater than 5, then we will round it and the value will be 0.169 into 10 power 3.

So, you see, what was the value we had before? x we had 0.1686 in 10 to the power 3. And after chopping, I represent it by xp. So, the xp that came out is 0.168 into 10 power 3. And xr if I write rounding, it comes out to be 0.169 into 10 power 3.

So, you can see that these values are zero. If we write zero and it becomes 90, then this value that comes in between. So, I can write from here that x will be greater than x p but less than x r in this case. Why? Because the value of x p has become less than x. That is, it was 86 or it remained 80. And what is the rounding off doing? It is not doing 9. So, here 90 has come. Right?

So, this rounding, I told you that you may either have to pay ₹20 or you may have to pay ₹21. So, it depends on what our values are. So, in chopping, just chop and leave it like that. Brother, this chopping has come. Okay? So, let's do rounding. So, we can do rounding like this. We can do chopping like this. Okay?

So, now as you might have done. If we see the value of pi, the value of pi is 3.14159265359 and so on. This value will go on. So, this is the value of pi. And the value of 22 by 7 is what we have. So, you can think that its values, pi and 22 by 7, if we see, till here it is the same but after that it changes. Okay?

So, this value will come. It is coming 3.141 and this is coming 3.142. So, from here we can say that in this case, the value of pi is less than 22 by 7. This is confirmed. But if we work up to two digits, then the value of both is the same.

So, if we do this, then I can write here that if we work up to two digits, up to two digits, then we can take pi as equal to 22 by 7. This means that we can use the value of 22 by 7 only when we are doing small calculations. Like we do in schools or in eleventh, twelfth. Even there we take the value of pi as 22 by 7 easily. And after that we do the calculation.

But if we have to do high performance computing where we have to use a lot of digits, then we cannot take the value of pi as 22 by 7 because there are errors in it. So, the errors will increase going forward

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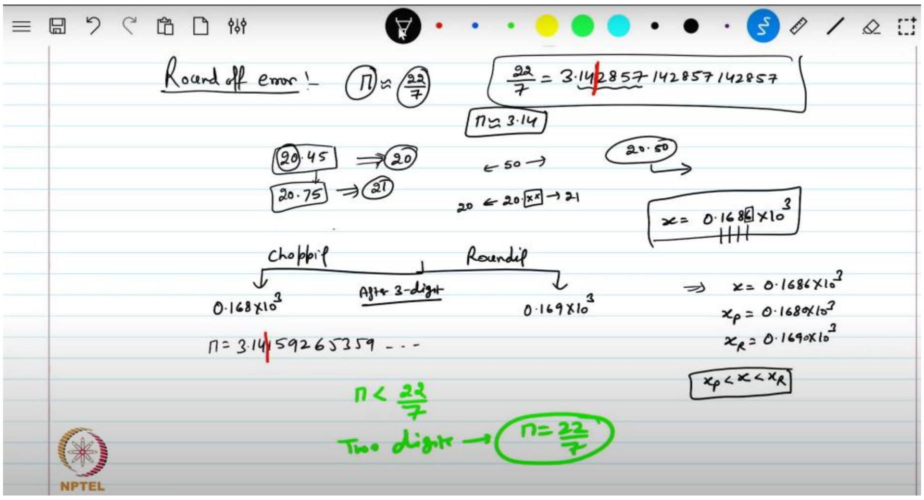

So now we have to see how to do this. What is happening in chopping? What is happening in rounding? So let's see all these things. Okay, so if we have a number x as 0.d1d2d3…. dn dn+1……dk up to here into 10 to the power some exponential, so I wrote it in the normalized form. So our first job will be to write it in the normalized form. Okay, so now see, what I have to do now is to round it after n digits. So, our main job in this is to do rounding after n digits.

So, there are two types of rounding. We have defined one as rounding off and one as chopping. So how do we show it? We have defined chopping. There is no problem in that.

Now how to round it? So, see, what do we have to do? n digits. So this is our digit. Take it till here. Okay, so we have to chop and round here that is truncate it. We have stopped this value. Okay, "truncate" means we have stopped it. Now after stopping it, what we have to do is check how we can stop it.

So, firstly, the first one comes. If the dn+1 is less than 5, then what will happen to us? The rounding off number will come. So, in this, we write no change in the value of dn. There will be no change in the value and it will remain the same. So, the number that we get, the rounding off number will come 0.d1d2….dn into 10 to power e. So, it will be saved here and will stop here. We will use this value.

Second one, if dn+1 becomes greater than 5, as the problem is at 5. So, if it is more than 5, then what will our number be? Then the dn will become plus 1. We will change its values. So, these values will be a dn +1. So, our number will be x star in this case. That 0.d1d2….(dn +1). Its value will increase by one. So, we know that it will become a bigger number if it is greater than five. What do we mean? We are giving 21 rupees to the shopkeeper.

The third one, what will happen if this dn+1 becomes 5 ? So, this has to be checked. S,o in this case, two cases will be created. Now I will write it like this. Let's take two cases. Let's take two cases.

The first case comes. If dn is even, means 0 2 4 6 8, take it like this. So, we will make no change in it. We will leave it as it is.

And if dn is odd, odd means 1,3,5,7,9. Then what will we do with it? Increase by one. That is we will make it even. In even there will be no change, and if it is odd, then we will make it even. So, we will do this work. Okay.

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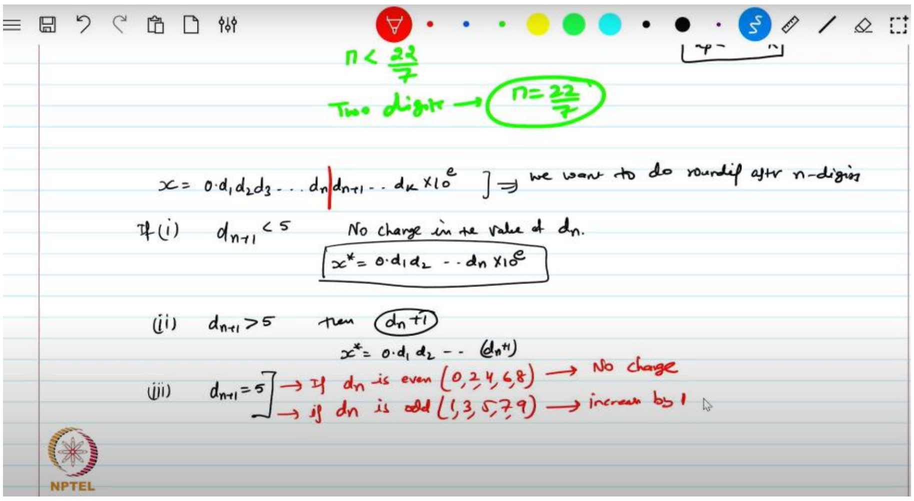

So, let's take an example of this. So, what will be its example? Like if I take a number, x, this is my number. I will write it 2.04567. This number came. Now first we got the number. Now I have to write that this number is in which form? It does not have any form. So, what will we do with this number first? We will normalize it. So, we normalized this number first.

So, after normalizing it, this number became 0.204567 into 10 to the power 1. If we multiply it by 10 power and then 10, then this number is in normalized form. So,what is our mantissa t? Our mantissa part becomes our main part. Now this part of the fraction is our mantissa, we already know it. And this exponent is fine. So, this exponent means we can do rounding anytime. So let me write it in normal form. So, I have written it in normal form.

Now suppose what do I do with it? Before that, I want to tell you one thing, that why are we doing this? There is a very important thing for that. There is a definition for that. We call it significant digits, significant digits. Okay, so what does significant digit mean?

Like we are doing a measurement. Suppose I am measuring nanoparticles. Okay, or suppose I am measuring the distance between two points. So, I know that the significant digit in it can be a centimetre or a millimetre as well. Now I am measuring the distance between two satellites. So, kilometre in it is also not significant.

So, this is called what are the significant digits in the calculation you are doing and which digits are not significant. So, what are the significant digits and how do we decide? So basically, if we write it in normalized form, then we write that all the digits are significant in the normalized form. If we have written in normalized form, then all the significant digits except zero, zero which we have written, used to fix decimals, except the zeros which are used for fixation of decimal points. Okay, this is called significant digit.

Now, for example, if we have a number, you gave us a number 0.002345, and asked what is the significant digit in it. So, we know that zero is not of that use. So, what did we do? We cannot tell like this what is the significant digit. So, what will we do now? We will write it in normalized form.

What will I do in normalized form? This x is like this. I wrote it as 0.2345 into 10 to the two power minus 2. I wrote it like this. Now we get to know that this number is between point 1 and one. So we wrote it in normalized form. Now we can say from here that these four numbers are all significant.

So, what does it mean? The four values in x are 2345 are significant. If there is a significant digit, then we got four significant digits in this number. So, if there are four significant digits, then these are numbers. So now we can take any number and we can round off or chop it.

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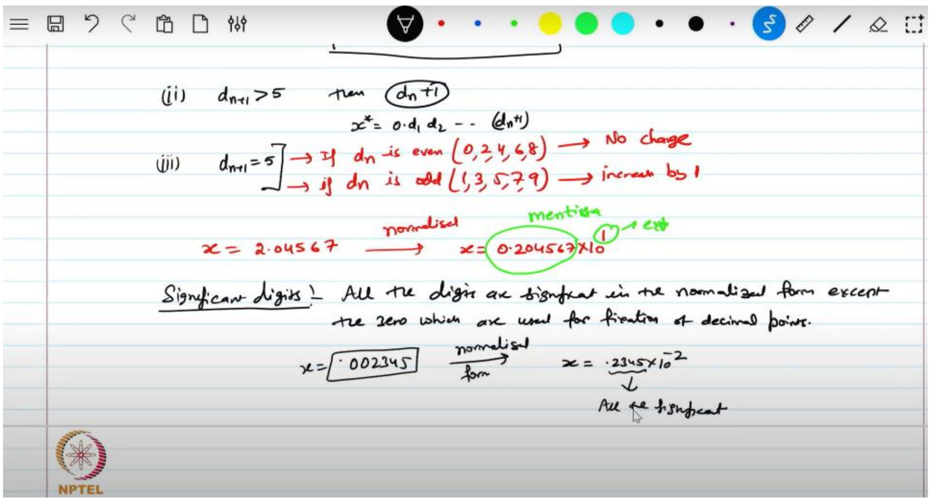

Now, for example, suppose I take the value of pi. Then the value of pi is 3.14159265. Now let me take this. Now, I do not need to apply the normalized form to it. If we are doing chopping, rounding, then if someone tells me to round it up to five digits, use this number and do not use it after that. So, what does it mean that I have been told that you have to stop here. The representation of this number will stop here.

So, I will stop it here. So, what I have to do is to stop this value here. So, I will go up to five digits and write it here. So, I will use pi and I will approximate pi. 3.14159 is okay because I had to go till here. Okay, so after that there is two, so no problem. I will use this value.

Okay, so in this we will say that the rounding that we did is rounding off after five digits. Now, if someone asks me to round to four digits, then we will round to four digits. So in that case, the values that we will get are approximate. So, I will write them here: 3.141. Now look here, if I have to stop in this case, then what will I do? Now this is the value, this is greater than 5, so I have to write 6 here.

So, I will take the value of pi now. If I want to round off after four digits, we can do this. Okay, so we can take the value of pi here as well. After even five, six, no matter how many digits we have, we can use the value of pi like this. Now, if someone tells me that you want to round off to 4, 5, 6 after the seventh digit, then the seventh digit, if you see, is coming here. And what is the value after that is 5? So the value of pi will come 3.141926 right here, after the seventh digit.

Okay, it will become the seventh digit because it is an even number. So, it will remain even, and if there is 5 there, then it will come here. This means that the value of pi has been told to us that you can use it in computation. So, we can use different values depending upon how much calculation our computer can do. Because you know that earlier computers had very little memory, so we were not able to do much calculation in them. So, we used to manage with the value of pi as 3.14 only.

But now that computers have high performance computing, their memory has also increased, their power has increased, so what is happening with that is that our calculations have become more precise. So, what can we do? We can tell things more accurately, that we can tell in science where the satellite will reach after 10 years. Because you know that some satellites have been sent to far off places, which have been launched. So, what happens there is that the calculations need very large calculations.

We need high performance calculations. The values that we have in it are its large digits, and we use these values in calculations. So, the one that evolves the most is the rounding or chopping error. This is used the most. So now the main question is how to do this. If we have any method, what will we do in future? We will make iterative methods. So, what should we write in iterative methods? That we get rounding off after four digits or three digits. What will it mean?

So, we can define this. So, I will give a small example. So how do we define it? Suppose we have a number x. So, we have rounded it and from there we have x star. So here x - x star is the modulated value. So, we will call it rounding error or error due to the rounding off. This is an absolute error. Basically, we can write it as absolute error because of rounding.

So, because of rounding off, we will get an error, that is for sure, we are going to get an error, right? So, if we will get an error, now suppose we have x star. So, if I have x star, this is my 0.4387, this is a number x. So, what do we have to do? Let our x be... what did we do? We rounded off to four decimal places. Okay, this was ours. And let x be rounded off after four digits. And after rounding, we got x star. The number that came out was x star.

So now we have to see what can be x in this case. You will see, if I have x, this is 0.43874, then this value will come. Then, if we do rounding on all of them, then we will get this value. Or else, the x that we have can be 0.43866, and here we have 7, 8. If I round it off, then it will become 7. Even if it is 7 , even if it is 8. If it is not there, then also it will be 5. Then it cannot happen because what will happen after 5 is there? It is an even number, so it will remain even, right?

So, in 5, if it can happen that if I have this value, then it is possible that my x will be like this: 0.43865. Not 86. If it is there, then it will not be there, okay. And if it is there, then it will become 8. Let this also not happen. So, this is also not possible. We have cut off this possibility. So, this is not possible. So, this can happen here. What does it mean? That our x can be this. This can be 0.4387 or 8 will increase by 7.

So, I write this as 0.43865, because it is not equal. Then it will be greater. And from where will it become less? 0.43875. Okay, so we have seen that 0.43865, I am taking it from here. It is not equal to the sign. It is sure that this will come to us. And if this comes, then it will be greater than x, and this value will decrease. I have told here. Okay, so this value which will be in between, now I will calculate it: x minus x star.

So, what did x minus x star do? We minus this value from it. So, it was 65, and it was 70. So, if you minus it, then this value will come to -0.00005. And this value came to us: 0.00005. Okay, so it means now we rounded it to four digits. So up to four digits, zero came. See, and this 5 came here. And this 5 came. So, from here I can write that x minus x star, modulus, absolute value is less than half into 10 to the power minus 4. I can write it as minus 4, okay.

And I can say, it is 0.5 into 10 to the power minus 4, and it had to go up to four digits, okay. So, if we have to round to four digits, then it means, if I write this in computational, then from here we will have automatic rounding to four digits, okay. This error was there. I can write this x minus x star, if I define it as 0.5 into 10 to the power minus 4, okay, and give something in x, then the x star will automatically be rounded off to four digits and we will get the values.

So, what do we do when we find the roots in scientific computing? We do not know what it is. So, what do we do when we round off the values, which are truncated values? Where do we have to stop the code? When the value of the solution of the code or the error in the root is less than something, it will stop there.

So, what do we have to do? Suppose we are finding the solution of an equation, its root, then what is happening in the root is that its values are coming out iteratively. So, suppose if we know the exact root value, then what will we do? We will define the exact root minus the iterative value, which is approximation, less than this. Then we will get the root until it gets accurate to four digits. So, this also means that the x and x stars will be same up to four digits. After that, the change will come, okay.

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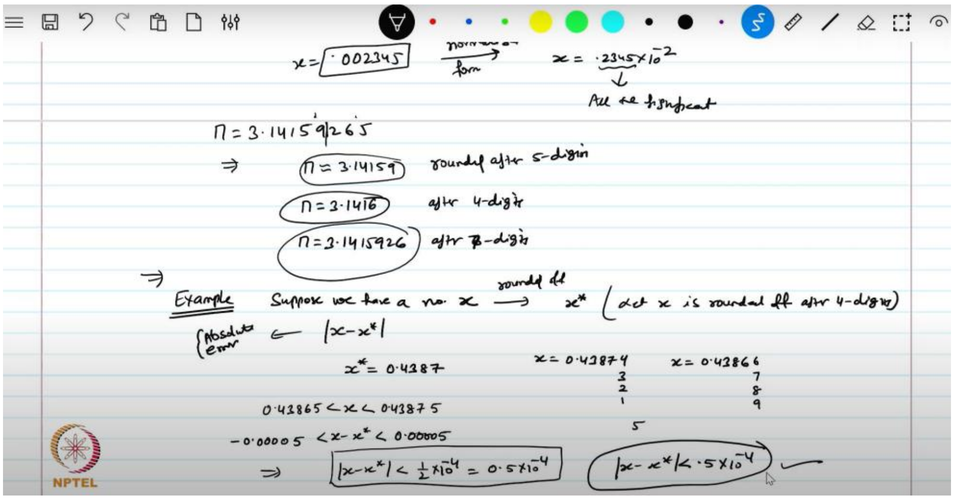

So, we call it rounding like this with the help of 0.5 into 10 to the power minus 4. We can do that. So, in this we will say that x is rounded to the four decimal places, and the maximum rounding off error is 0.5 into 10 to the power minus 4. So, we should always remember this thing. So let me write here that if x is rounded to a decimal, then what will we have to write? x minus x star, the rounded number that we get, we will have to define it like this.

We can also do equal to 0.5 into 10 to the power minus n. So, if we get this error, okay, then we can find out from here. So ,we will use this criteria, and you will see later that this thing which is coming, we will call it tolerance. Tolerance is given so that where does it have to be terminated. Your iterative process will stop. So, it will keep going on for us.

So, we will round off in this way, and we will do chopping in the same way. We have come to know that rounding-off error is increasing or decreasing the elements. Chopping is always reducing it, right? But rounding can decrease the values of the elements as well as increase them. So, after doing this, we get some errors which we define.

Now we have been told about absolute error. What is absolute error? Absolute error is $|x-x^*|$. Its approximations are called absolute error.

The second one is relative error. So, what is relative error? $|x-x^*|/|x|$, which we wrote. So, what did we do? We divided it by $|x|$. So, we will say that it is the relative error. So, what can we do from here? We can define relative error. We can also take the relative error with respect to x^*, and we can also do this as $|x-x^*|/|x^*|$. We can also define this.

So, we are taking this modulus so that if it is negative, then it will give a positive value; otherwise, it will remain the same. In this, we are only interested in seeing its value, right?

So, in the same way, we can also find out the percentage error. We will multiply it by 100 and get the percentage error. Then we will get the percentage error from there. If this percentage error comes, then the relative error into 100 will become the percentage error. Okay?

So now suppose we have something. I took a number. Let's take an example. We had a number x, it was 0.6348954, this value. And what did we do? We rounded it. Suppose I first did the chopping, okay? So, I got x_c^*. I wrote 0.6348 this is chopping error. And what did I do? After that, I rounded it after four digits.. So, I wrote x_r^* this is the rounding error. The rounded number will come out to be 0.6349. Now, if it is 8, then this is greater than 5, so It's value will be 9. I have calculated its value.

Now $x - x_c^*$,how much will this chopping error be? The chopping error will come to be 0.0000954, this value. Subtract this from this, simply, right?

What does it mean? That next we have zero. Basically, it became 8000, and this was 8954. This is a big number. So here comes $x - x^*$ come Okay?

Now, what do I do? $x - x_r^*$ and give how much is that. Oh, now xr is, if we see, then this is 9000, and that is 8954. So, it will come out negative. Okay?

So, I take the modulus. Now, you see this error was because of the chopping error. This error is so much as compared to the error, in this case, we can write that it is quite high, and it means that it is reasonable. So, we will compare the two.

The chopping error in this is quite high for this number, and the relative error for this number is quite low as is compared to the chopping error. So, we have done this.

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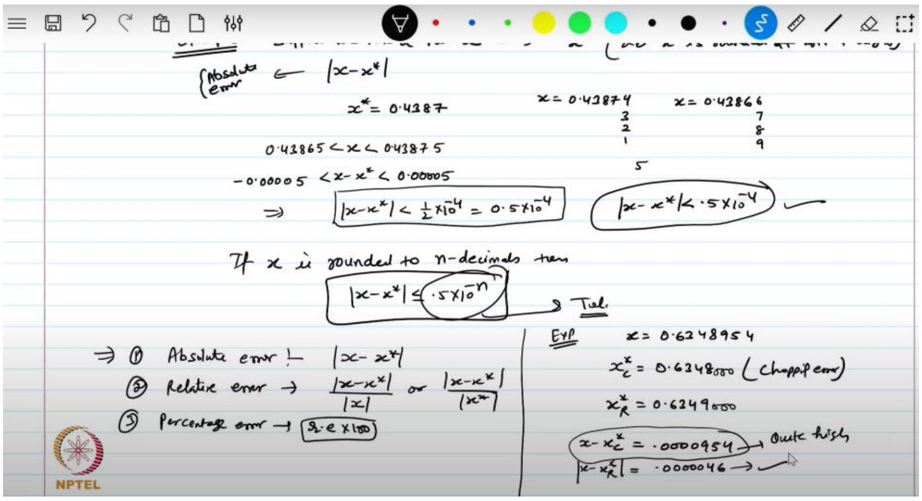

Now what will we do? We will try to find the relative error. So, in this case, if I find out what the relative error is, okay?

So, the relative error , if we find out the relative error in this, then you can see that I find it in chopping. Because it is positive, so there is no problem. So, I will find it with respect to x.

So, you can see that 0.0000954 divided by x, what we have is 0.6348954. If we divide this, it comes to 0.0001502.

And if we see the percentage error, then the relative error in this will be, if we multiply it by 100, then there is this much percentage error: 0.015%, if we chop the number.

And similarly, if we do rounding, then if we see the relative error with respect to rounding, then we will do $|x - x_r^*|/|x|$. So if we calculate it, then you will see that the relative error that we have if you solve it using the calculator then it will come out to be 0.00000724.

So, if we do it in percentage, then what will happen in percentage? Relative error into 100. So, the value that we get will come out to be 0.000724%.

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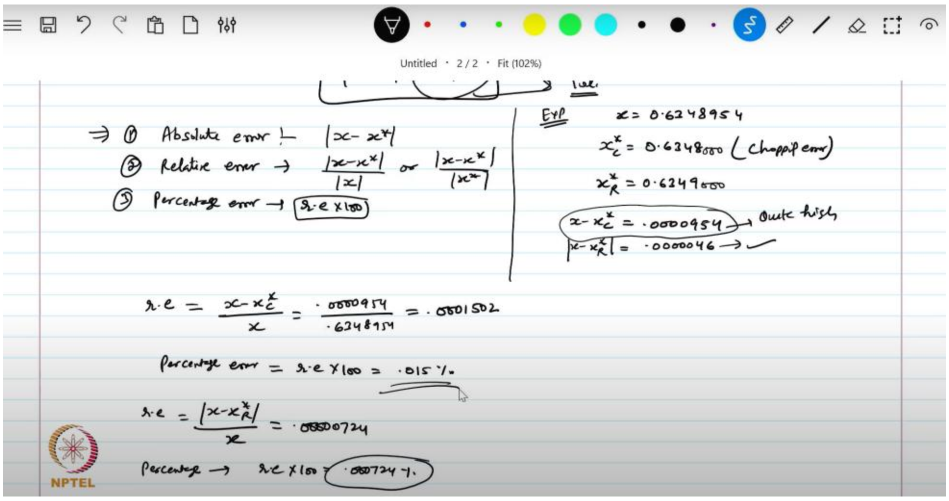

So, this error is very low as compared to this percentage. So, in this case, the computer says that the chopping error is quite high as compared to the rounding error. So, we can say this. And after that, it will happen, so in the same way, we have errors which are of different numbers, and we can calculate their errors. So, these are the errors that we have discussed, what are rounding error, chopping error, and significant digits, how can we normalize a number?

So, these are our basics, which can be done in every computation because we have to find out the absolute error in it as well as the relative error.

So, today we have done some basics about how errors always evolve in our computations. Truncation, whenever a number is truncated we have discussed that today. So, we will move ahead from this in the next lecture.

So, thank you for listening to this lecture.