Advanced Mathematical Methods for Chemistry
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Module - 06
Optimization, Constrained Optimization
Lecture - 01
Maxima and Minima, Taylor Series

So, now we will start module 6. In module 6, I will be discussing about Optimization and Constraint Optimization. Now, optimization means finding the extremum values of the function like the maxima and minima and what I want to do in this module is to show how you calculate maxima and minima for different kinds of functions, especially functions of several variables and how you calculate these when there are certain conditions on the function. So, this is something that is very practical and you will use it a lot and it is good to have a formal understanding of these things, so that it will make lot of analysis easier.

So, let us first start with the first lecture, where I will be talking about maxima and minima of functions and I will talk briefly about Taylor series.

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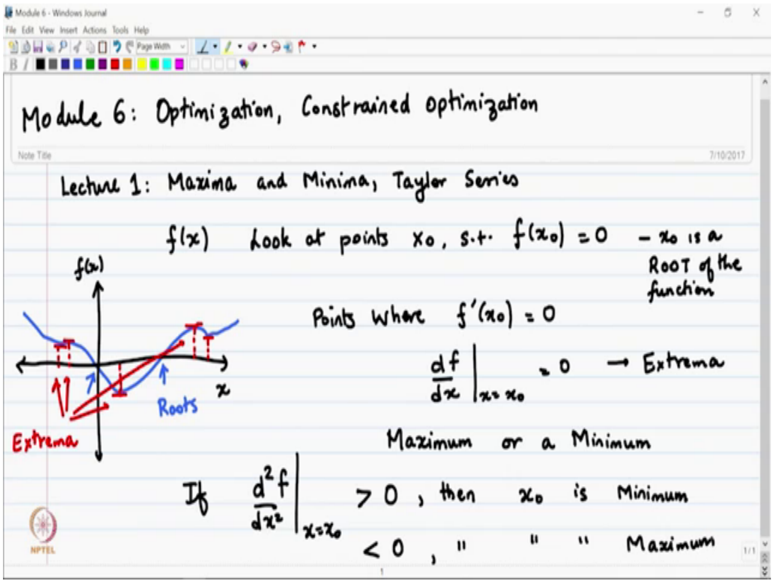

So, suppose you have a function f of x. If you look at points x 0, there could be many points x0, such that f of x 0 equal to 0 and then, that point is called a root. Then, x 0 is a root of the function. So, what you say is that if I just show it graphically, so if this is my x and a plot f of x on the y axis, now if f of x has a form that looks like this, then the places where these points are what are called the roots. Now, you could also look at points. So, points where f prime of x 0 equal to 0 that is f prime of x 0 is df by dx evaluated at x equal to x 0 equal to 0.

So, these are called extrema and geometrically df by dx represents the slope. So, these are points, where the slope of the function is 0. So, the slope of function is a local tangent. So, clearly here the slope if you look at this part, the slope is not 0, where the function becomes flat. That is why the slope goes to 0. So, these are the various points. So, if you look at this point here, the slope is 0 because the function is locally flat here and the slope is 0.

Similarly here the slope is 0. So, these are the various places where the slope is equal to 0. So, these points are called Extrema. Now, if the slope is 0, your function can go in this way then it goes through a minimum value at that point x 0. If it goes the other way around, then goes through a maximum value of that at that point. So, it can be either a maximum or a minimum. So, the value of the function is maximum or minimum at these extrema. So, now, what is the condition for maximum or minimum? So, if d square f by dx square at x equal to x 0 is greater than 0, then x 0 is a minimum and this is for an extremum. So, if you already have an extremum extrema point that is the first derivative is 0. If the second derivative is greater than 0, then it is minimum. If it is less than 0, then x 0 is maximum.

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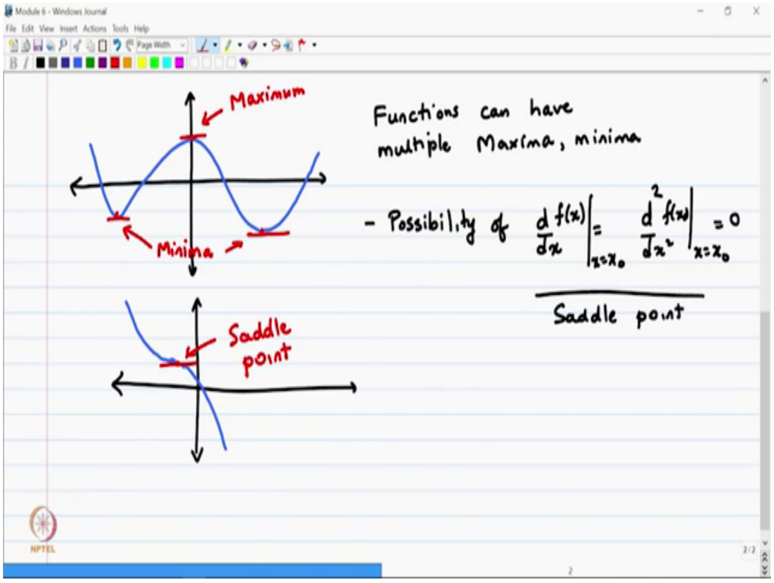

So, these are fairly well known expressions, but it is good to think about them geometrically. So, what is happening is that. So, let me just show function for simplicity. I will just take a few points. So, now, what you see is that at this point the slope is 0, the function is locally flat. This point also the slope is 0; this point also the slope is 0. So, these are the three extremum points and clearly this is a maximum, these two are minima. You can easily verify the second derivative, the rate of change of slope. So, as you come to the minimum, the slope is negative and as you cross the minimum, the slope becomes positive. So, the slope changes from negative to positive. So, the rate of change of slope is greater than 0 whereas, at a maximum, the slope changes from positive to negative. So, the rate of change of slope which is the second derivative is negative. So, this is fairly well known. Now, a few points I want to make of function. Functions can have multiple maxima minima. So, they can have more than one maximum or minimum.

The next point I want to make is that it is also possible is, this is not the only possibility. So, there is a possibility that of t by df d by dx of f of x equal 2 at x equal to x 0 is equal to d square by dx square of f of x at x equal to x 0 equal to 0. So, the first derivative is 0 and the second derivative is also 0. So, then what happens if the second derivative is also 0? So, it is not a maximum, it is not a minimum. So, what is it? So, this is called a saddle point and as the name says this has a slightly different shape. So, a saddle point I will just show one saddle point. So, if you have a function, the slope is 0 at this point. Now, if you gone up, it would have been maximum, it would have been a minimum, but what is happening is it goes down this way. So, now at this point the slope is 0, but also the second derivative is 0.

So, this is called a saddle point. So, these are ideas of a maximum minimum saddle points. So, these are all extremum values of the function and these turn out to be extremely significant in various applications. So, it is very good to have a good understanding of these points.

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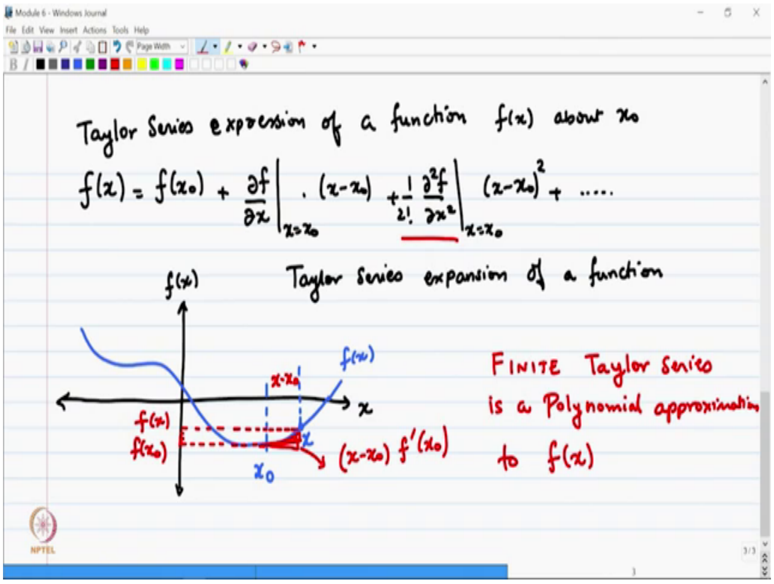

Now, let me show as I will explore the nature of functions a little more, bit more using the Taylor series. How you know the Taylor series? The usual, the standard Taylor series or Taylors formula series expression of functions. So, you write f of x, you write it as f of x 0 and x 0 is some point plus the function f of x about x 0. So, about the point x 0. So, then you will write dou f by dou x evaluated at x equal to x 0 times x minus x 0 plus dou square f by dou x square 1 by 2 factorial evaluated at x equal to x 0 times x minus x 0 square plus and so on. This is an infinite series.

Now, the significance of this Taylor series so, this is called the Taylor series. It goes all the way to infinity series expansion of a function. Now, let us look at what we are doing in this function. So, let us look practically at what we are doing when you are evaluating a Taylor series. So, let us look at it graphically. So, if you have x and f of x and let say you have some function that looks like this. So, I have just shown this is my f of x. Now, when you are doing a Taylor series, what you are doing is you are writing an expression for this function and let us take for simplicity let me take this as x 0. If you have a point x, what you are writing is, you are writing the value of the function at this point as f of x 0.

So, what is f of x 0? The first term is f of x 0. So, this is f of x 0. Now, this should be your f of x. Now, what you are doing is, you are writing this function as f of x 0 plus you are taking the slope at x 0 and multiplying it by this difference in x. So, this is x minus x 0. So, now if you take the slope and multiply by the difference, then let us say the slope is something like this. So, this is a term x minus x 0 times f prime of x 0. So, I am just writing f prime of x 0. For this expression, df by dx evaluated at a x equal to 0 and just calling it f prime of x 0. So, this slope multiplied by this will give you this additional increment. So, what you are doing is, you are writing f of x as f of x 0 plus this much. So, this is the small interval that you got which I am showing on this axis so clearly. That is not all. Then, you add a second term which is related to the second derivative times some other times x minus x 0 square, ok.

So, that is like a quadratic expression for this. So, that might give you something around here. So, the next thing is to use this quadratic term. So, that will get you closer to the function and you keep doing this, you keep doing more and more terms till you get closer and closer to the function. So, what is important is that finite Taylor series is a polynomial approximation to f of x. So, if you truncate the series at a finite point, what you are doing is, you are approximating it by a polynomial. So, f of x may or may not be a polynomial. It might have exponentials, it might have sins, it might have logarithms, it might have all kinds of functions, but what you are doing is, you are approximating it by a polynomial. What we are doing is, you can also think of it as graphically going closer and closer to the function using various properties of f if you want to do a Taylor series.

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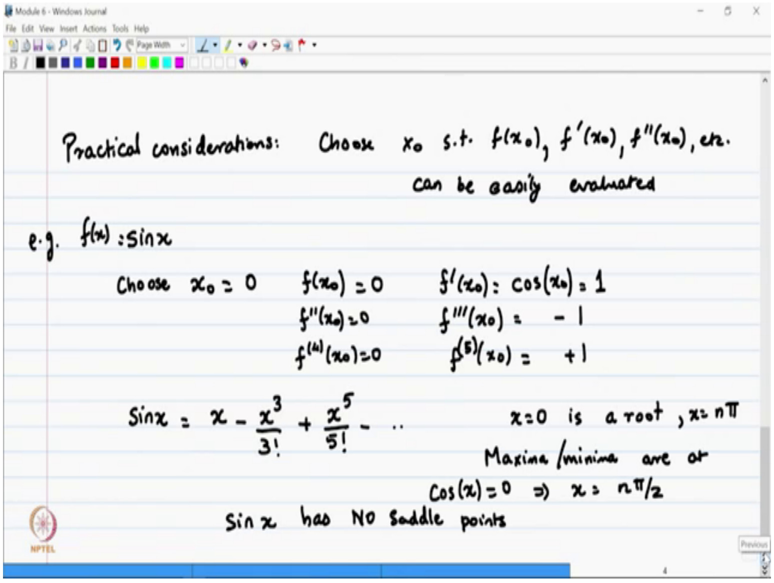

So, practical considerations in Taylor series considerations choose x 0, such that f of x 0, f prime of x 0, f double prime of x 0 etcetera can be easily evaluated. So, for example let us take sin x example.

So, let say f of x equal to sin x. So, now I will do a Taylor expansion of this. So, I mean you might know the expression, but let us try to work it out. So, choose x 0 equal to 0. So, then f of x 0 equal to 0 that is sin 0. Now, f prime evaluated x 0 equal to derivative of f of x is cosine of x 0 and you put x 0 equal to 0 cosine 0 equal to 1 f double prime of x 0. So, second derivative is derivative of cos x is minus sin x. So, this is minus sin x evaluated at x equal to 0 is 0 f triple prime of x 0. Now, you are taking three derivatives. So, when you take the first derivative, you will get cosine. You take the second derivative, you will get minus sin. Take your third derivative, you will get minus cosine of x 0 and then, you put x 0 equal to 0. So, then minus cosine of 0 is minus 1. Well, sort of see what will happen, so f of x 0 it will be 0 f phi of x 0.

So, the fifth derivative evaluated at 0 will be plus 1. So, we will go from my plus 1 minus 1 plus 1 and so on. So, I can write my Taylor series in the following form sin x is equal to sin of 0 is 0. So, f of x 0 is 0; f prime of x 0 is 1. So, you have 1 into x, x minus x minus 0. So, you just have x and then, you have minus. The odd term is the even terms are 0. So, the next odd term will be x cube divided by three factorial plus x phi divided by phi factorial and so on. So, this is the Taylor expansion of sin x. Now, this is very useful because you can look at limiting behaviour, you can compare with polynomials you can do all kind of things. So, Taylor expansion is a very practical and useful thing to do. It also you know when your derivatives go to 0, you can immediately identify maxima and minima also.

So, you can clearly see that x equal to 0 is root and you can also see that maxima and minima are at cosine of x equal to 0 implies x equal to n pi by 2 and you can also see that there are other routes for various multiples of pi. So, it is x equal to n pi. So, the maxima and minima of function and you can also have saddle points or functions. Now, in this case, you do not have any saddle points. So, sin x has no saddle points which is very obvious because you cannot have both. First derivative and the second derivative go to 0. This is one of the features of sin x.

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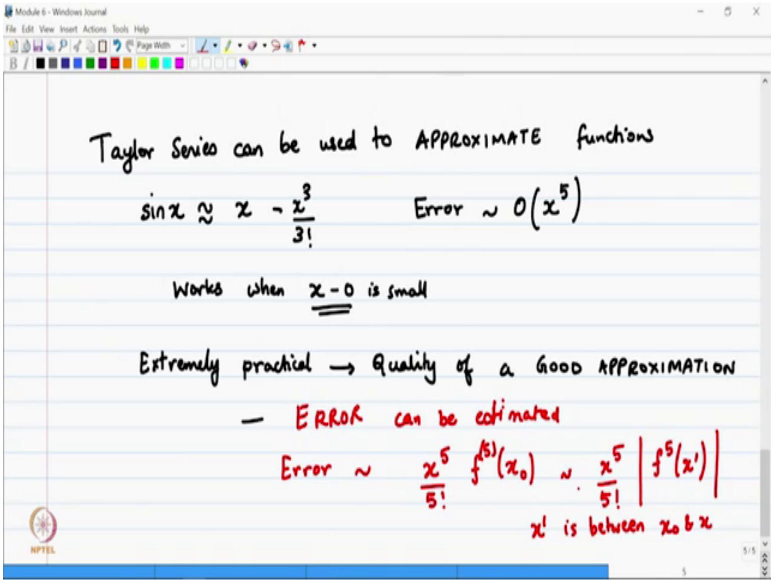

Now, Taylor series is also used through as an approximation method can be used to approximate functions. So, for example, I can write sin x is approximately equal to x minus x cube by three factorial. I can just write sin x is this.

So, when I write this approximation, then the error. So, this works when x minus 0 that is x minus x 0 is small and the error term is of order x raised to 5 because the first term in the error has x raised to 5. This is one way to look at approximation of functions. So, this works when x minus x 0 is small because when x minus x 0 is small, then each of these successive terms will have higher and higher powers of x and they will get smaller and smaller. Now, Taylor series can be used to approximate functions and you can also get an estimate of the error. So, this is extremely practical because this is a quality of a good approximation. What is the quality of a good approximation is that the error can be estimated. You cannot calculate the error exactly because if you know the error exactly, then you know the function, but what I am saying is even if you do not know all the higher derivatives, you can still approximate it. So, the error can be estimated by the approximation method.

So, this is the quality of a good approximation. In fact, we can put a more practical estimate of the error. So, the error goes as it is x raise to 5 divided by 5 factorial f, the fifth derivative of x 0. So, this is kind of an estimate of the error. So, what is typically what you say is that the error when you make this approximation goes as something like x raised to 5 divided by 5 factorial times. You just evaluate the fifth derivative at some point x prime and when you take the absolute value. So, x prime is between x 0 and x. So, that is how you do it and x 0 is 0. So, you say that the error is somewhere here because this is the leading term in the error. You can have higher order terms also. So, we can say that we can put an upper bound for the error in this way. So, I will conclude this lecture here.

In the next lecture, we will start looking at functions of many variables and we will first look at Taylor series for functions of many variables, then we look at how you look at extremum points for functions of many variables.

Thank you.