Advanced Mathematical Methods for Chemistry

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Module - 06
Lecture - 02
Taylors Series for Functions of Several Variables, Maxima and Minima

So, in this lecture, we will try to extend the ideas of Taylor series and maxima and minima to functions of several variables. So, I would like you to recall what we learnt about functions of several variables. When we said that when we talked about vectors, we saw when we take derivatives of functions of several variables, the gradient was used to denote directional derivative. So, the gradient was related to a directional derivative and it was also related to the direction where the rate of change of function is maximum.

Now, you might think that you know functions of several variables have maxima and minima for these functions and the answer is yes, you can very much have maxima and minima for these functions of several variables. In fact, it turns out to be extremely useful in various analysis to know what are the maxima minima and what are these sometimes called the critical points, where the function or its derivatives, any of its derivatives goes to 0.

So, the analysis of the functions and its critical points is actually something extremely used before we get to analyzing the maxima and minima. Let us try to see what the Taylor series expansion will look like for a function of several variables.

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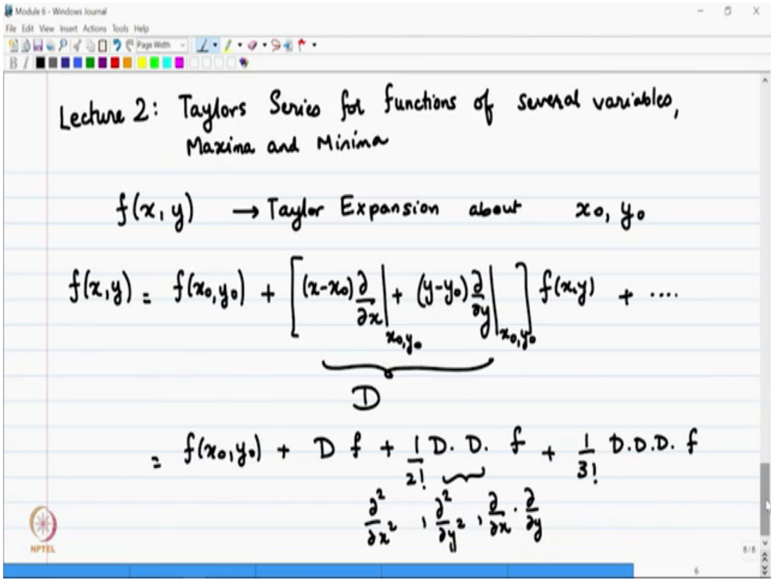

So, we start with a function. Now, you have a function of xy. Let me write this as you want a Taylor series, Taylor expansion about x 0 y 0. So, now a point is specified by these two coordinates; x 0 and y 0. So, you want to do a Taylor series about x 0 y 0, ok.

So, I will just write the final expression and then, we will try to analyze it in more detail. So, f of x, y I can write as f of x 0 y 0 plus. So, x minus x 0 dou by dou x plus y minus y 0 dou by dou y and this derivative is evaluated at x 0 y 0. This derivative is also evaluated at x 0 y 0 of f of x y.

So, this is the first term and I deliberately wrote it in this form. So, I mean if you want, if you can bring the f in front of both these, but basically I wrote this as this common. See if you had only a function of x, then you just have the first term. If you had only a function of y, you just have the second term. Now, here the only difference is, this is replaced by a partial derivative and there are two terms. You add both of them. Let me call this whole operator as D operator.

So, what I will write this as f of x 0 y 0 plus d f plus d d f divided by 2 factorial plus 1 over 3 factorial. So, d d d f and so on. Now, I just wrote this in short notation. So, df is just this whole d. You can think of D as acting on f. So, d acting on f will give me this whole term. Now, what I do is, d acting twice, ok.

So, I take the derivative twice and then, I put x equal to x 0. So, operate by this whole thing. So, notice that this will have terms like d square by dx square. It will have terms like d square by dy square. It also have cross terms, where you have d by dx into d by dy. So, it will also have these kind of cross terms. This is what the Taylor series expansion looks like for a function of several variables.

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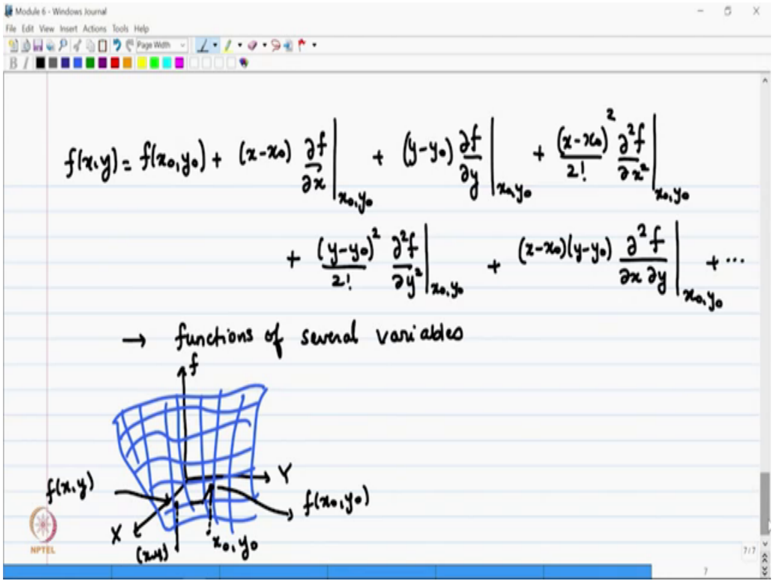

Let us write down a couple of terms. So, suppose I have f of xy is equal to f of x 0 y 0 plus x minus x 0 dou f by dou x evaluated at x 0 y 0 plus y minus y 0 dou f by dou y evaluated at x 0 y 0 plus x minus x 0 square divided by 2 factorial dou square f by dou y square dou dou x square evaluated at x 0 y 0 plus y minus y 0 square by 2 factorial dou square f by dou y square evaluated at x 0 y 0 plus x minus x 0 times y minus y 0. There will be two terms, ok.

So, therefore, that will cancel the two factorial and what I have is dou square f by dou x dou y evaluated at x 0 y 0 plus higher order terms that in all three derivatives. So, this is what your Taylor expansion of a function of two variables will look like and similarly, you can extend two functions of several variables, ok.

So, this is what the Taylor series will look like and let us look at it geometrically. What you are doing? So, here you have a function of two variables and as we said earlier if you have a function of two variables, this is y and this is x and then, I plot my f here. Then, f typically looks like some sort of the function might have another value here. So, this might be f of x y.

So, this is f of xy, this is f of x 0 y 0. So, what you are doing in this Taylor expansion is, you are using the slopes. Now, when you take dou f by dou x, there you are keeping y fixed. So, we are moving only along x. So, taking the derivative moving only along x, you move along this. Then, the other derivative you take only along y. So, you move along y direction and then, similarly you take second derivatives and you take cross derivatives and so on, ok.

So, that is how you are trying to approximate this function in terms of the value of the function at x 0 y 0. So, that is about Taylor series for a function of several variables. Now, what about maxima and minima? What about let say extrema?

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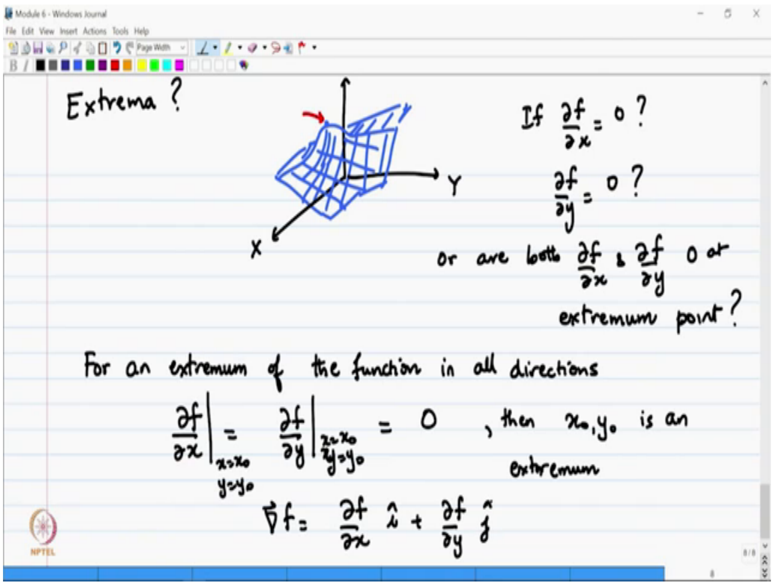

Now, clearly you can have extrema even for a function of several variables. For example, just graphically if I show, you could have something that looks, so this is x and y axis. You could have a function that has like a little, it has a little extremum point, right where it goes through a maximum. You could have the surface of the function go through some maximum value and here clearly you can see pictorially that the function is maximum here. F of x is maximum, ok.

So, what would be the characteristic of an extrema? So, dou f by dou x equal to 0 or f dou f by dou y equal to 0 or are both dou f by dou x and dou dou f by dou y 0 at maxima at extremum point.

So, what should be the condition for the extremum? For an extremum of the function, I will say in all directions. So, if you have a point that is extremum in all directions, then you should have all derivatives be 0. So, dou f by dou x at x equal to x 0 equal to dou f by dou y at x equal to x 0 y equal to y 0 x equal to x 0 y equal to y 0 equal to 0, then x 0 y 0 is an extremum. You know that dou f by dou x and dou f by dou y are basically components of the gradient.

So, you know that del f is equal to dou f by dou x times i plus dou f by dou y at j. So, now if you look at del f evaluated at x 0, y is 0, ok.

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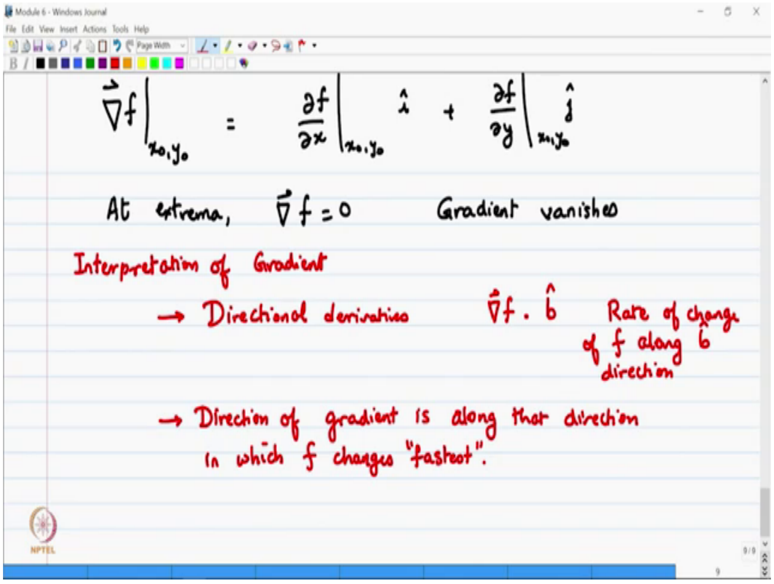

So, this is nothing, but dou f by dou x evaluated at x 0 y 0 times i plus dou f by dou y evaluated at x 0 y 0 times j.

So, that means at extrema grad f, let me put a vector sign grad f equal to 0. So, the extrema grad f has to be equal to 0. So, the maximum and minimum of a function of multi dimensional of many variables will have gradient equal to 0. So, gradient vanishes. So, it goes to 0. This is a very practical observation. You remember the two interpretations of gradients?

So, interpretation of gradients we learnt in terms of directional derivatives. So, grad f dot b hat, this is the rate of change of f of f along b direction. So, suppose you want to find how the function is; what is the rate of change of function along b direction, along some direction, then you take the gradient multiplied by the unit vector in that direction, ok.

The second thing is gradient, so the direction of gradient is along that direction, where along that direction in which f changes fastest. That means, it means along the steepest. So, if you look at this graph, gradient will point along the direction, where the rate of change is fastest. So, it could be that it is much slower in this direction and much faster in this direction. So, the gradient will point along the direction where the function changes the fastest.

So, now you can say that if the gradient vanishes, then the derivatives along any direction will go to 0 and obviously, the direction of gradient changes fastest, but the rate of change of f along any direction is actually 0 because the gradient is 0. These are two things that you will notice immediately, ok.

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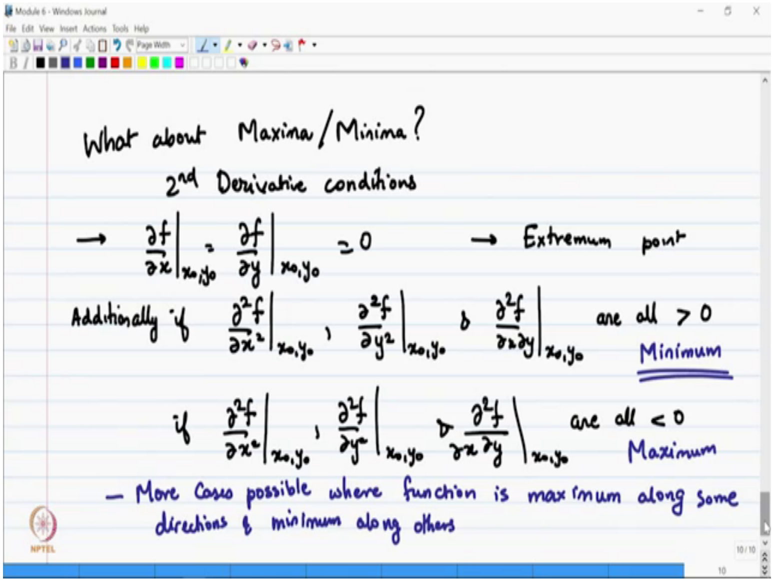

For a function of many variables, each of the derivatives has to be 0 along an extremum point. What about maxima or minima, what about maxima slash minima, our second derivative conditions?

So, what we say this is fairly obvious. So, if you have dou f by dou x at x 0 is equal to dou f by dou y at x 0 y 0 equal to 0, then this is extremum. Additionally if second derivative, if all second derivatives and dou square f by dou x dou y evaluated at x 0 y 0 are all greater than zero, if they are all greater than 0, then the function is minimum.

Now, on the other hand if dou square f by dou x square by dou y square and are all less than 0, then clearly it is maximum along all directions. Now, you could also have additional cases. So, more cases possible where function is maximum along some directions and minimum along others; so, one of these derivatives might be greater than 0, one might be less than 0 and so on, ok.

So, you could have also had things like that where function need not be maximum along all directions or minimum along all directions, but it can be maximum and minimum along certain directions. You could also have cases where you have things like saddle points. So, the function is maximum along one direction and a saddle point along another direction. So, all these things are possible and you know you should really imagine these by trying to visualize certain functions and try to see how a maxima looks. So, if it goes like this, then you know that it is maxima. It is a maximum at that point.

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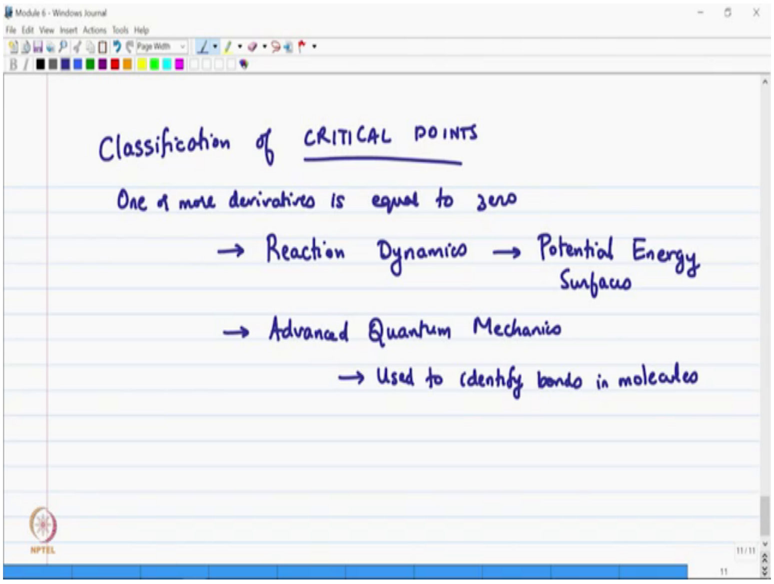

On the other hand, if it goes like something like this, then you know that ok you have points where the derivative is 0, but it looks like it is maximum along this direction, but it might look like minimum along one direction, but maximum along another direction. This is classification of critical points.

So, these are points where one or more derivatives is equal to 0. So, these are points where one or more of the derivatives is equal to 0. So, the classification of critical points, this is very important. Let say in various areas like in reaction dynamics, for example, if you are doing and if you are looking at the potential energy surfaces, so you want to know maximum, you want to know what the transition state is. It is maximum along one direction and minimum along all the other directions and so on.

This is one place where we use, this is another place where you use it as in I would say advanced quantum mechanics. So, this is used to characterize, used to identify bonds in molecules. So, we look at the electron density. So, you look at the electron density which is a function of several variables and you try to look at where its derivatives go to 0. So, when you identify all those critical points and looking at the nature of the critical points, you can identify various points and you know places where electron density changes, ok.

So, I will conclude this lecture here. In the next lecture, what I will do is, I will try to look at the process of optimizing a function of many variables and in particular look at something called constrained optimization. How do you do an optimization, when you not only optimize the function, but you also have certain external constraints, ok.

Thank you.