Advanced Mathematical Methods for Chemistry
Prof. Madhav Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Module - 06
Lecture - 03
Critical Points of Functions

In today's lecture, I will be talking about the classification of critical points of functions and I will be elaborating on some of the topics that we did in the last two lectures. We saw how to understand maxima and minima of functions in very simple terms. Now, you might have functions that are slightly more complicated than the simple functions that we looked at. So, it is good to have a general idea of how to classify the critical points of functions. So, I will first talk about functions of a single variable and then I will talk about functions of two variables, but you can extend these arguments to functions of more than two variables also, ok.

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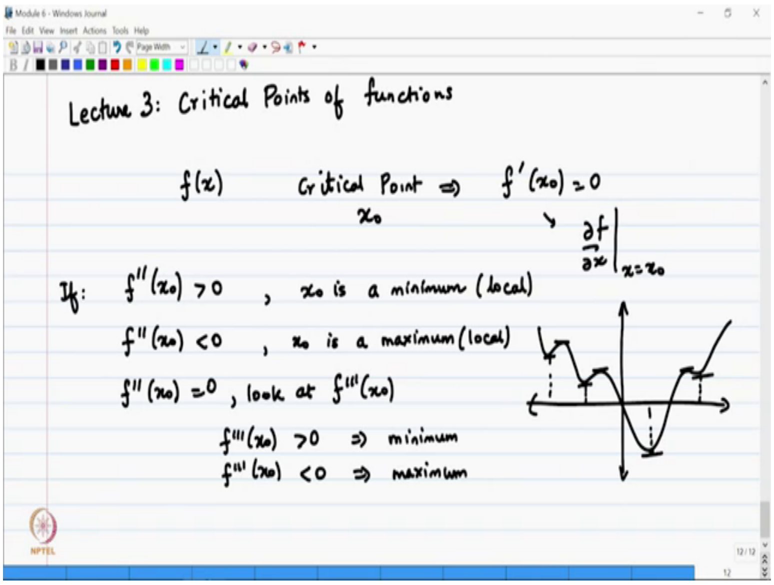

So, let us look at a function of a single variable. So, if you have f of x now a critical point. So, critical point implies f prime of x 0 equal to 0. So, then x 0 is a critical point. So, x 0 becomes a critical point if the derivative at x 0 equal to 0. So, f prime of x 0 is a short notation for dou f by dou x evaluated at x equal to x 0. Now, that is a critical point. Now, there can be different critical points. So, to know nature of critical point, you look at f double prime of x 0. So, if f double prime of x 0 is greater than 0, then x 0 is minimum and we should emphasize that this is local minimum suppose to a global minimum. So, suppose you have a function what we said is that your function can have several minima.

So, it can have a function like this. So, now each of these points is a local minimum. So, each of these points, the derivative is 0. Similarly you can have local maxima also. So, each of these is local maxima. Now, the global minimum of this function is right here. This is the minimum value of the function, but the first derivative will be 0 for each of these. Each of these points will also satisfy minimum conditions. If f double prime of x 0 is less than 0, then x 0 is maximum and again local maximum if f double prime of x 0 equal to 0, then there are a lot of things that are possible.

What you have to do is look at f triple prime of x 0, ok. Then, you use the same condition. So, what you will see is f triple prime of x 0 is greater than 0 implies minimum, local minimum. F triple prime of x 0 less than 0 implies local maximum. This is if the second derivative is 0. If the second derivative is 0, then you have to look at the third derivative. If the third derivative is 0, you look at the fourth derivative, ok.

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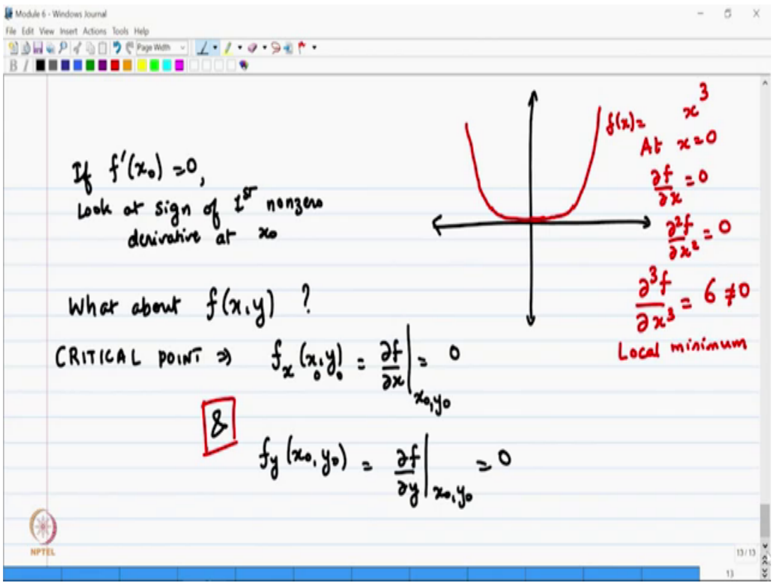

So, now what are the kind of functions that can have a second derivative 0, but a third derivative. So, you could have a function something like that comes down and then, it goes almost flat for sometime. So, it goes flat enough that the second derivative is 0 and then, it goes up again. Suppose you just take a function like x minus x cube, ok.

Now, you know I will just say x plus x cube or just x cube for that matter. Now, at at x equal to 0 dou f by dou x equal to zero, no space here. This is f of x equal to x minus x cube. So, at x equal to 0 dou f by dou x equal to z equal to 0 because dou f let say 1. I just say x cube. Let me just put it as x cube. So, let us just take x cube for example. So, at x equal to 0 dou f by dou x is equal to 0 dou square f by dou x square equal to 0 and dou cube f by dou x cube equal to 6 not equal to 0. This is at x equal to 0 at x equal to 0 at x equal to 0 dou f by dou x is 3 x square because x equal to 0 if that is 0 dou square f by dou x square is 6 x which is equal to 0 at x equal to 0, but the third derivative is not 0, ok.

So, clearly this is a local minimum. So, the point is you have to look at the first non-zero derivative. So, if f prime of x 0 equal to 0, then look at a sign of first non-zero derivative at x 0 and then, you can identify maximum or minimum. That is a condition for identifying maximum or minimum. Of course, if all derivatives are 0, then the function is just constant. So, that is a trivial case which I won't bother about.

So, this is what you do with functions of single variables. Now, what about functions of many variables functions of 2 variables? So, the definition of critical point implies f x of xy equal to dou f by dou x equal to at x 0 y 0 at x 0 y 0 equal to 0 and f y of x 0 y 0 and this is very important. Both the condition should be satisfied. So, this is very important which is dou f by dou y at x 0 y 0 equal to 0. So, that is the condition for the critical point.

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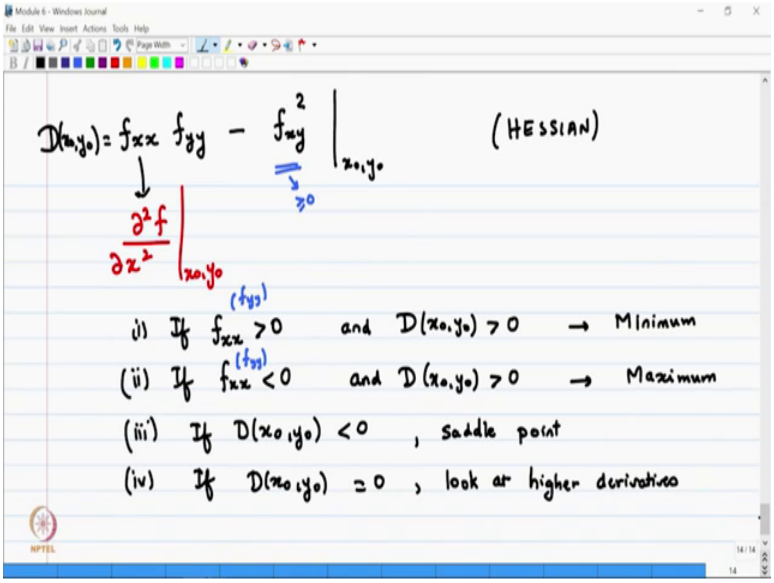

Now, you can ask the same question when is it a maximum, when is it a minimum? So, in order to identify maximum or minimum of a function of many variables, what you do is you define fxx fyy minus fxy fxy square and call this as d of x 0 y 0. So, you are evaluating this at x 0 y 0. All this each of these derivatives. So, this is nothing, but dou square f by dou x square evaluated at x 0 y 0. So, this quantity D, this object D is sometimes called the Hessian. Now, the way you classify the critical points is you say you look at the first case and if fxx is greater than 0 and d of x 0 y 0 is greater than 0, then this is minimum and it is a local minimum again. Everything is local minima.

Now, the second case is if fxx is less than 0 and d of x 0 y 0 is greater than 0, then it is a local maximum. The third case is, if d is greater than 0, you can have two cases where ff fxx is greater than 0 or it is less than 0. Now, notice the second term in d xy. This is always greater than 0, this is greater than 0, greater than or equal to 0 because it is a square. So, if x x if if d is greater than 0 and fxx is greater than 0, then automatically fyy has to be greater than 0. Similarly, if d is greater than 0, again if fxx is negative, then fyy also has to be negative. So, you can use the same condition even for fyy. This is only if d is greater than 0. The third case is if d of x 0 y 0 is less than 0, then it is a saddle point. If this is less than 0, then this point is a saddle point.

Now, notice each of these can be greater than 0. Fxx fyy can all be greater than 0 and fx fxy can also be greater than 0, but if this d is less than 0, then it becomes a saddle point.

The fourth case is if d of x 0 y 0 is equal to 0, then we have to look at higher derivatives. So, what I want to say is that you know you have to look at look at various partial derivatives in order to decide what kind of critical point you have. So, now let me just illustrate this with a very simple example of a function and we will look at this function and we will identify and list all the critical points and then, we will classify them, ok.

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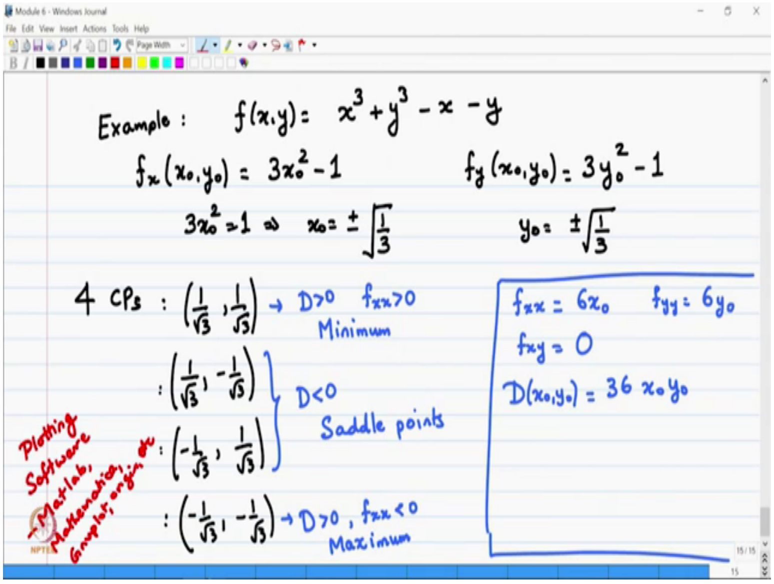

So, let us just take a simple example. So, suppose I take f of x y is equal to x cube plus y cube minus x minus y. So, what are the critical points? So, if you want to identify the critical points, what we will say is f x of x 0 y 0 is equal to x 0 square minus 1 and fy of x 0 y 0. So, the first term is independent of y. So, the second term will give 3 y 0 square and then, this term x won't contribute the derivative with respect to y be minus 1.

So, now at the critical points 3 x 0 square equal to 1 implies x 0 equal to plus or minus square root of 1 by 3 and y 0 equal to plus or minus square root of 1 by 3-4 critical points. What are the four? So, the first one is 1 by root 3, 1 by root 3, the second one is 1 by root 3 minus 1 by root 3, third one is minus 1 by root 3, 1 by root 3 and the fourth one is minus 1 by root 3 minus 1 by root 3. This is the value of x 0 and y 0. So, you have these four critical points.

Now, let us try to classify them. So, let first calculate fxx. So, I will write here and this fxx. So, first I will write the general derivative and then, I will substitute the critical points. So, fxx is equal to 6x 0, fyy is equal to 6y 0, fxy is equal to 0. So, therefore, now you can calculate d of x 0 y 0 is equal to 36 x 0 y 0. So, now in the first case and the fourth case, d is greater than 0.

Now, if you look at the second if you look at fxx for this, so fxx is greater than 0. So, this is clearly minimum ere fxx is less than 0 and this is maximum and these two points have d dx for these two points d less than 0 and these are saddle points. So, just by looking at the function and taking its derivatives, we identified where it is maximum, where it is minimum and which are the saddle points of this function, ok.

Now, you can go ahead and if you want you can actually plot this function using standard plotting software. So, you can use plotting software especially in multi-dimensional plots. So, full of plotting software such as Matlab Mathematica, Gnuplot, Origin etcetera; using any of these plotting software, you can actually plot this function and you can actually visualize some of these maxima and minima. So, I encourage you to do this and this will help you get a better understanding of these critical points. So, I will conclude this lecture here.

So, in the next lecture we will talk about Lagrange's method of undetermined multipliers.

Thank you.