Advanced Mathematical Methods for Chemistry
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Module - 06
Lecture - 04
Lagrange's’s Method of Undetermined Multipliers, Optimization, Total and Partial derivatives

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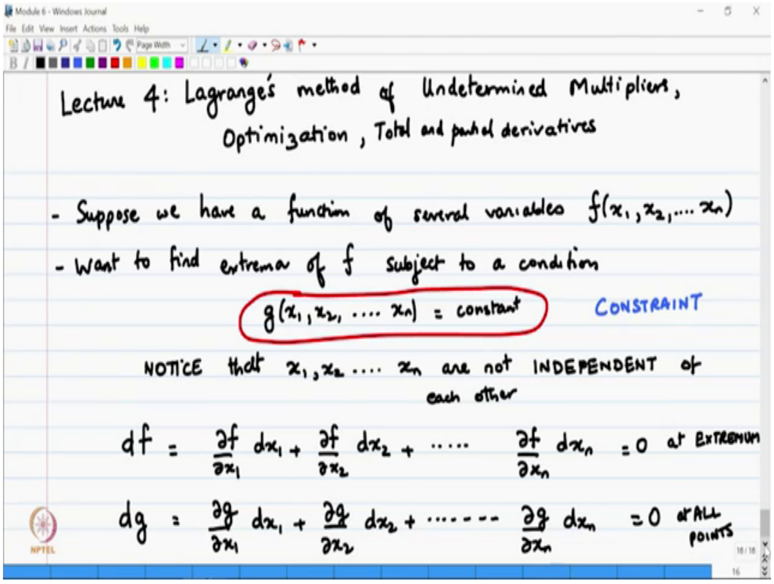

So, in this lecture which will be the 4th lecture of Module 6, I will introduce the method of Lagrange's undetermined multipliers which is a way of finding the extremum, the maxima or minima of functions which satisfy a certain constraint. So, this is a very powerful method and it is very widely used to both in quantum mechanics and in statistical mechanics. What I will show the basics of the method and then, will explore certain topics which are related to the foundations of this method.

Let us get to the basic task at hands. So, suppose you have a function. We have a function of several variables and we denote it by let say f of x 1 x 2 up to xn. Now, we want to find extrema. Extrema means minima or maxima of a function of f subject to condition. The condition is we write it in this form g of x 1 x 2 upto xn. Let us say equal to constant or I can only take the constant to the left I can say equal to 0.

So, this condition refer to as a constraint to we have this function of several variables and we want to find the extrema of this function subjected to this condition. We look at an example I mean they are the most common example of these are basic geometry. You might be asked to find out very cubical problem. You must find the volume of parallelo piped, find the shape of a parallelo piped that has the largest volume for a given area, ok.

So, these are the kind of questions, geometric questions that can be easily answered using this that are usually of this form. Suppose you want to find that subject to that constraint, then what we notice is, before we give the solution, we notice that x 1 x 2 up to xn are not independent of each other. That is because of this condition. There is a relation between x between all this x 1 x 2 up to xn, ok.

So, they are not completely independent. So, this is something that should be kept at the back of your mind that you know these variables are not completely independent. Now, in this case we are treating them as they were independent, but then we will have to put this constraint. So, now if this constraint was not there, then you would use the expression for total derivative.

So, df as dou f by dou x 1 dx 1 plus dou f by dou x 2 dx 2 plus dou f by dou xn dxn. This is the total differential of f. The differential change in f is written in this form and at the extremum, this differential change should be 0 because each of these derivatives should go to 0. This goes to 0 at extremum. This is the condition that you have, ok.

Now, if you take dg. So, that dg now g is the constant. So, dg will also have to be 0, but I can write g also in a similar form equal to 0. This is 0 everywhere. This is 0 for all points. So, at all points, what this implies now remember this is little strange equation because when you define these partial derivatives, you are keeping all the other variable fixed, ok.

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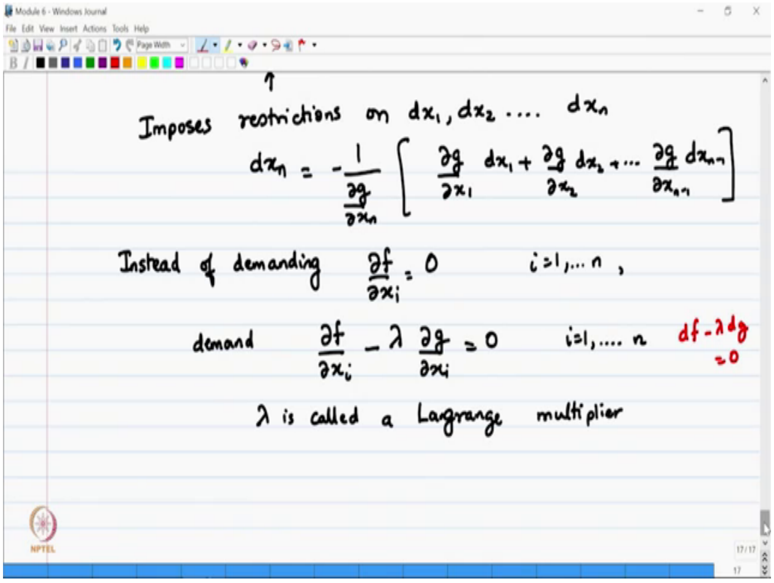

However, we already said that you know you cannot do this because all these variables are not independent of each other. Actually this condition we use this condition on dg to as this imposes restrictions on dx 1 dx 2 upto dx n. For example, you should have d xn is equal to minus 1 over dou g by dou xn times dou g by dou x 1 dx 1 plus dou g by dou x 2 dx 2 plus upto dou g by dou xn minus 1 d xn minus 1.

So, your d xn for example cannot be independently vary. It depends on all dx 1 dx 2 upto d xn minus 1. So, you cannot independently vary d xn according to the Lagrange's method of undetermined multipliers. So, what you do is the derivation of the method, but what you say is instead of demanding dou f by dou x 1 dou xi equal to 0 now for all i. So, i equal to 1 to n to n, ok.

So, you demand dou f by dou xi minus lambda dou g by dou xi equal to 0. Now, i equal to 1 to n lambda is called Lagrange's multipliers. Lagrange's multiplier you can clearly see that this should be showed true because all we did was we took the second equation here. So, we took this equation multiplied by lambda and subtracted it from from this equation, ok.

So, what we did is basically we did df minus lambda dg equal to 0. So, this is basically this condition and we look at it term by term. So, we look at it term by term and I mean there is a formal derivation which I am not doing, but basically this is the method, this is the basic idea of Lagrange's undetermined multipliers.

What you do is you take the constraint multiplied by a constant lambda and now, you have n equation. These n equations will help you solve for x 1 to xn. So, remember here it look like you have n equations, but actually these dx 1 dx 2 are not independent of each other. You cannot use that equation, this form here in this case when you used as Lagrange's undetermined multipliers, ok.

So, you have extra variable. So, let us now look at an example of how this works; very classic example and this is a typical geometric example.

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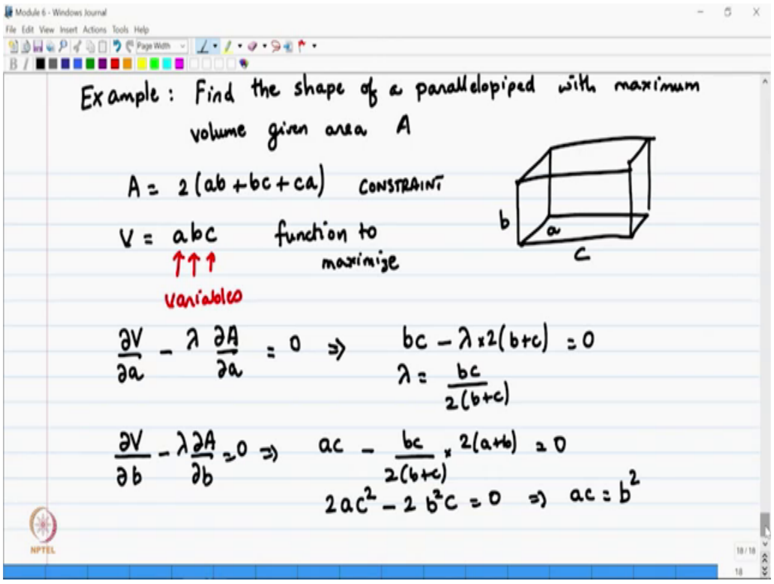

Find the shape of a parallelo with maximum volume given area A. So, for a given area of A of parallelo piped, find the shape of parallelo piped with maximum volume, ok.

So, what you do is just show you what this problem is. So, you have parallelo piped. A parallelo piped has three dimension. So, a b and c. So, these are the three sides, the length, breadth and width and height. Now, the area A is equal to twice ab plus bc plus ca. So, this is the constraint now volume equal to abc, this is the function to maximize.

When you do this, you will get a relation between ab and c and that will tell you what the shape of the parallelo piped is. So, we use a Lagrange's undetermined multipliers. So, now notice that variables are abc. The abc are your variables and they are not independent because of this condition dou v by dou a minus lambda dou a by dou a. This is equal to 0 implies what is dou v by dou a dou v by dou a is b times c minus lambda.

Now, dou a by dou a has now there are two terms with a. So, it is twice 2 b plus c equal 0. This gives you lambda equal to bc over twice b plus c, take the value of lambda and put it in the next equation dou v by dou b minus lambda dou a by dou b equal to 0 implies now dou v by dou b by this same argument, this will be ac minus.

Now, lambda is bc over twice b plus c. So, this will be twice a plus b, this equal to 0. You can expand this out. So, suppose multiplies twice b plus c, then I will get 2 abc and 2 ac square and I have minus 2 abc and 2 b b square c. So, I can write this as 2 ac square minus 2 b square c equal to 0 ac equal to b, b square equal to ac, ok.

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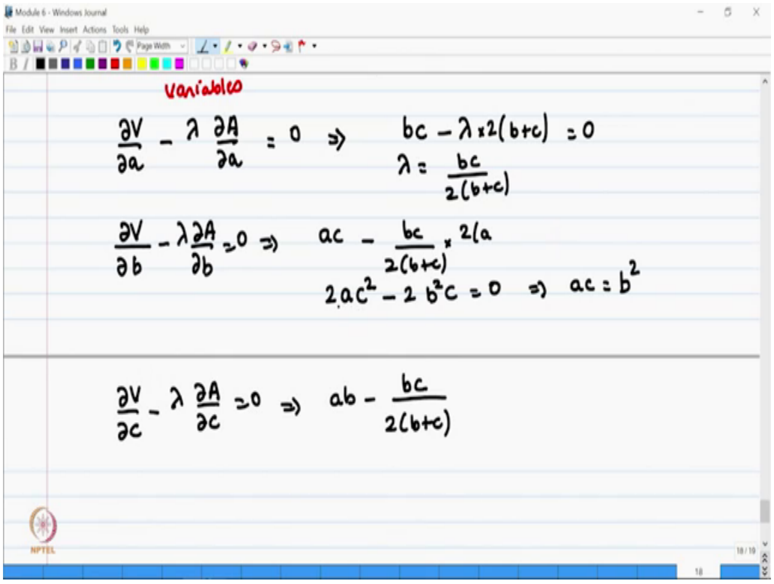

So, that is the constraint that you get from the second equation. Now, we still have one more equation. Suppose I use dou v by dou c minus lambda times dou a by dou c equal to 0. So, this implies ab minus. Now, I will again substitute the value of lambda bc over twice b plus c and I have just one correction dou v by dou b minus lambda time dou a by dou b equals to 0, ok.

So, this implies now if you take dou v v by dou b, you will get ac minus lambda. Now, dou a by dou b that will give me, let me substitute the value of lambda.

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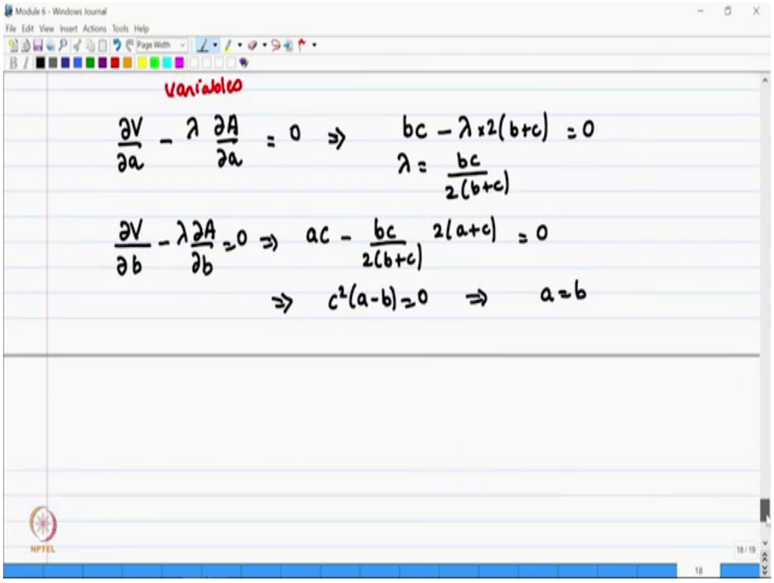

So, bc over twice b plus c, now dou a by dou b I can see that twice a plus c and this has to be equal to 0 and now, I have just multiply of b plus c. So, I cancel the two and I multiplied b plus c. So, what I will get is that the first term will be abc and here also the first term is abc. They will cancel and then, we will have ac square and you have bc square.

So, you have c square times a minus b equal to 0 and c square cannot be 0. So, that implies a equal to b and this is the condition.

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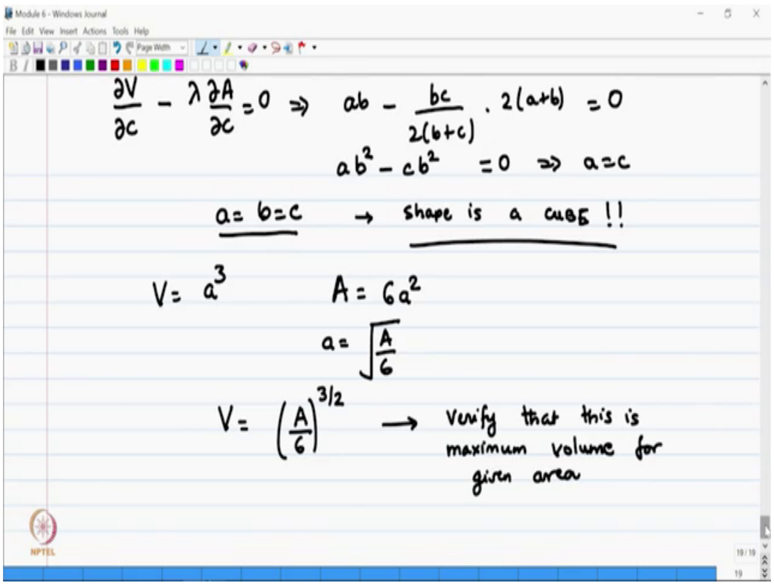

We still need to find out c. So, we will use third equation. So, dou v by dou c minus lambda dau a by dou c equal to 0 implies now will have ab minus what you had is bc over twice b plus c into twice a plus b equal to 0 and remember a was equal to b and we do exactly what we did last time.

So, what we have ab square and abc and you have ab. So, you have ab square minus the next term here will be cb square equal to 0 implies a equal to c. Thus, a equal to b equal to c. So, the shape is a cube. So, cube is that shape, maximize the volume for a given area. Now, how do we know it is a maximum and not a minimum?

If a equal to b equal to c v equal to a cube, now what about area? Area is basically given by twice a square into 3. So, that is 6 a square. At this point we do not know whether it is maximum or minimum volume. We just know that the volume is extremum. Now, if you want to check whether it is maxima or minima, then you have to take the second derivative and look at all those, all the constraints that we had that we had used earlier.

I can write a is equal to A by 6 under root and v is equal to A by 6 raise to 3 by 2. This is a volume that corresponds to an extremum and in fact, you can verify that this is maximum volume for given area. You can verify that you take any other choice for a, b and c which satisfies this given area and then, you will get lower volume.

So, I leave that as an exercise for you. So, with this I will conclude this discussion on Lagrange's method of undetermined multipliers and in the next lecture, we will work out some practice problems that use the technique of Lagrange's undetermined multipliers. Also, we use some of the other techniques that we have learnt in this module.

Thank you.