Statistical Thermodynamics For Engineers
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Lecture 10
Supplementary Video 2 Stirling Approximation and Lagrange Multipliers

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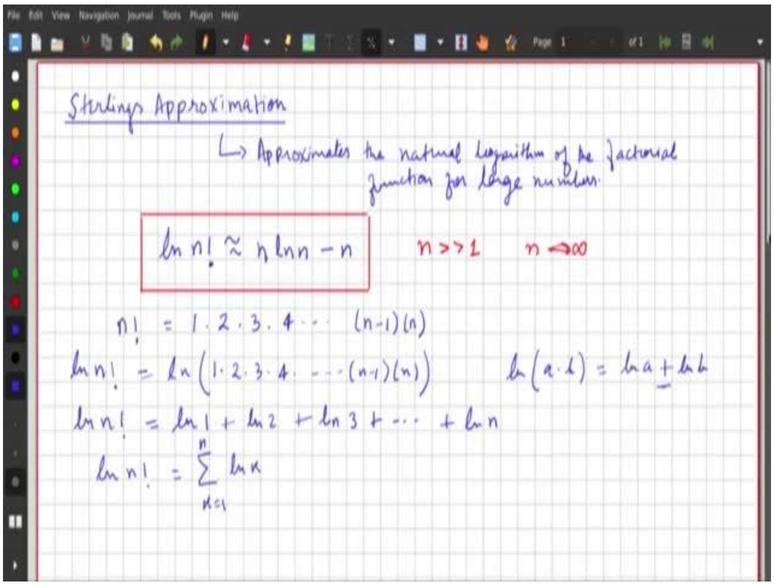

Welcome everyone to another session of supplementary videos and today we will be discussing a mathematical idea. So, we will begin with a very important concept that we use in statistical mechanics quite a lot and that is the idea of Stirlings Approximation, so, we will be discussing what Stirlings Approximation is all about. So, what Stirling Approximation basically as you can see think about this as an approximation and what it approximate is?

It approximates the natural logarithm, natural logarithm of the factorial function for large numbers. So, let me write down the Approximation first. So, let us say what Stirling Approximation says is? Take the log of n factorial this is approximately equal to n log n minus n so, this is what Stirling Approximation is all about. And this is valid this this result gets more and more accurate as n becomes larger and larger. So, this is valid for n much much greater than 1, the result becomes more and more accurate as n tends to infinity basically, this is what Stirling Approximation is.

Let us see how this comes about. So, if you think about n factorial function, so, what it is? Is basically a product of 1 into 2 into 3 into 4 dot dot upto n minus 1 into n this is a product of n natural numbers, and if you take the logarithm of this you get log of n factorial which is basically log of the product of all the natural numbers let us say till n.

And if we use the identity that log of the product of two quantities is equal to log we can write it in this so, the product becomes additive. So, if we apply it for all the n terms, this we can write this equation as log of n factorial equals log 1 plus log 2 plus log 3 plus dot dot dot log n or we can write this in a summation notation. The n factorial is equal to sum overs this is you see log of a running index some let us call that key and that key runs from 1 to n. So, till here you see that this is no approximation till here because we just use the definition of factorial function and took the log of both sides and wrote it in summation notation.

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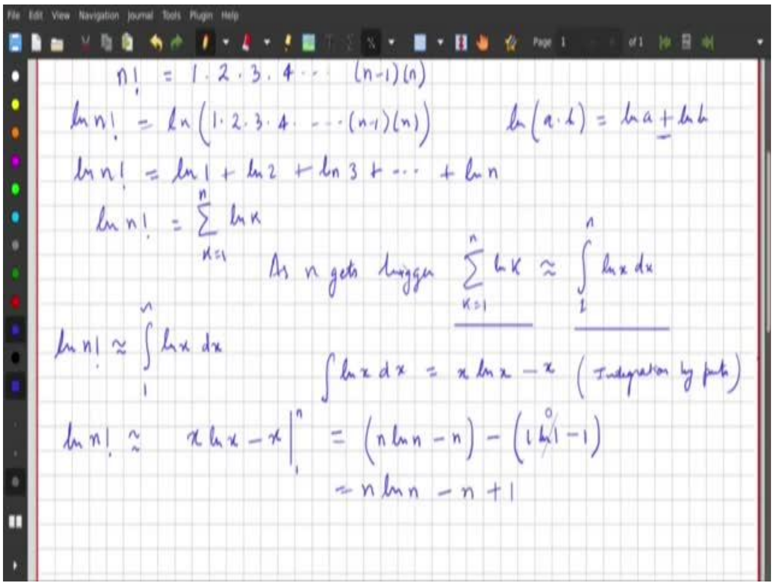

Here comes the Approximation that we want to do. So, as n gets larger as n gets bigger the sum k is equal to 1 n log k can be approximated by the integral of log x dx from 1 to n. So, this is where the Approximation comes through. So, what we do is, we approximate the sum by an integral and this Approximation becomes better and better as n becomes larger and larger.

So, if we write that then we have log n factorial is approximately equal to the integral of 1 to n log x dx, using the fact that the integral of log x dx is x log x minus x and this comes from integration by parts, integration by parts, and so, if we note so this is if you see this is the indefinite integrals, so, if we use this here for our definition, it becomes log of n factorial is approximately equal to x log x minus x limit from 1 to n. If we use this limit this will become n log n minus n minus 1 log 1 minus 1 and since log 1 is 0, so this becomes n log n minus n plus 1.

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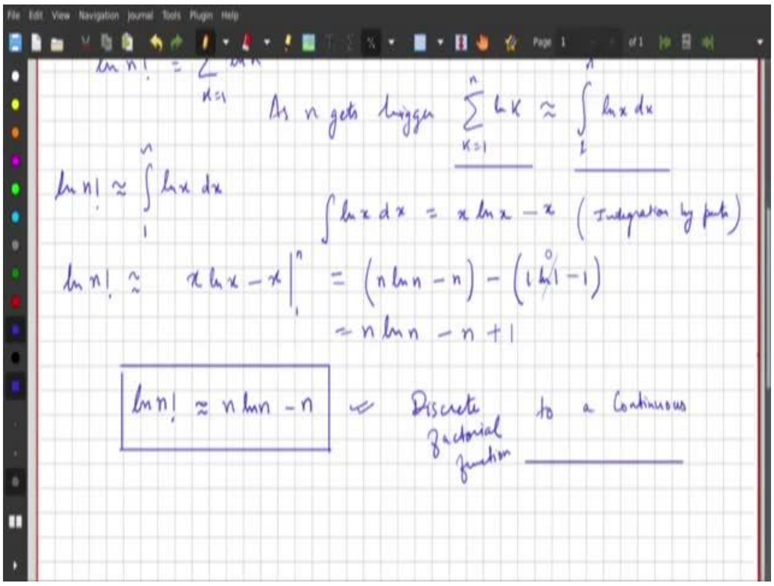

And since as n gets larger and larger, this one becomes basically negligible. So, therefore, we can write log of n factorial is approximately equal to n log n minus n. That is what Stirling Approximation is, yes, and this is used. This is the most frequent expression that we use in statistical mechanics, by the way where we because in statistical mechanics, what we do is always we start by counting the possible number of possible ways. So, we are doing a lot of permutations and combinations and there we have lot of factorial functions.

So, this expression, what it does is it converts the discrete factorial function to a continuous one and the moment we do that, what happens is we can use the rules of calculus, and that makes a lot of that makes the job a lot easier, because it is always easier to handle smooth functions rather than discrete functions. So that is all about Stirlings Approximation, it is used quite a bit in statistical mechanics.

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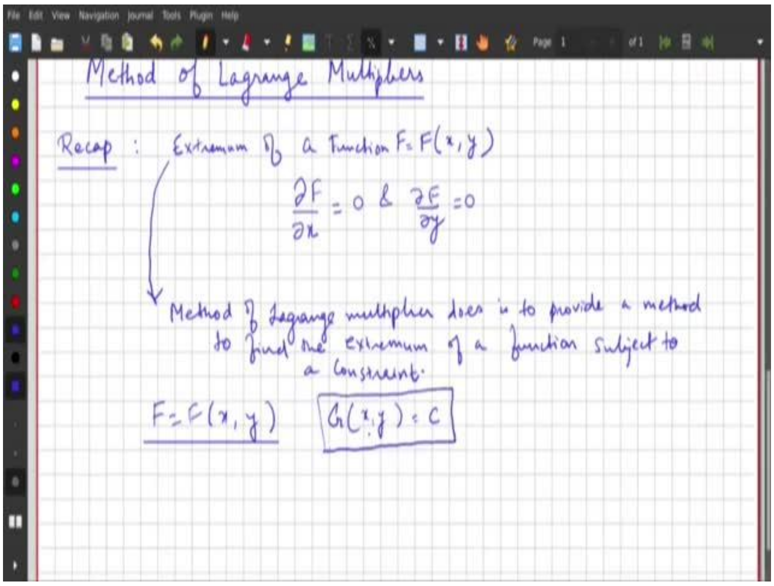

Now, we move on to the next concept of today and that is the idea about method of Lagrange multipliers. This is the next topic for today. That is a method of Lagrange multipliers and what this method is used for. So to understand this, let us let us recap our understanding of let us say if you want to find out the extremum of a function, let us say the extremum of a function, let us say of two variables just for example, it could be extended to arbitrary so, this is a function whose extremum we want to find out and if you want to find out the extremum of this function, the condition that we use is partial f partial x equals 0 and partial f partial y equals 0.

What the method of Lagrange multiplier does is? Is basically extend this idea of finding out the extremum of a function either maxima or minima, but subject to a constraint. So, what this method of Lagrange multiplier does, Lagrange multiplier does is to provide a method to find the extremum of a function subject to a constraint, subject to a constraint. So, that is what the method.

So now, when we are having a function for example here, so now what we want to do the general problem is let us say we want to find out the extremum of this function F of x y subject to the constraint that the function let us say G of x comma y equals constant, we want to find out the extremum of this function, but there is a constraint equation between x and y. So x and y are no longer so, like there is a relationship between x and y that needs to be satisfied.

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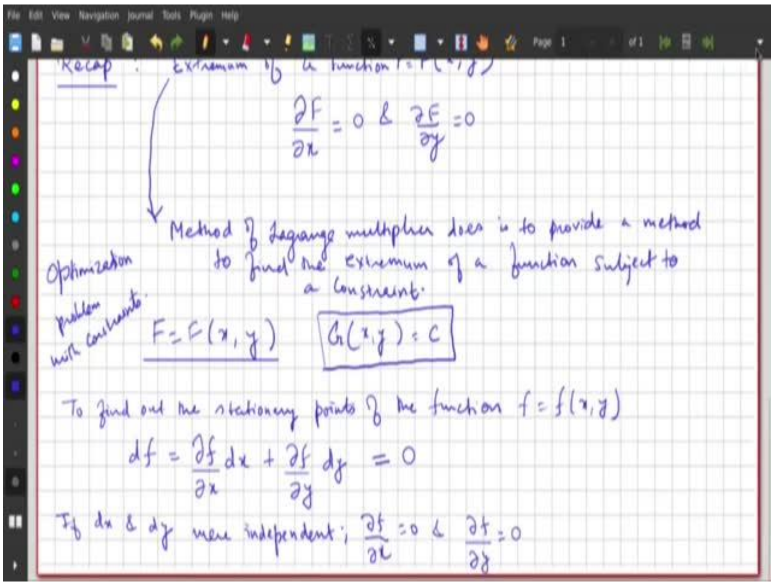

And this belongs to the class of an optimization problem or condition. So what we are actually solving is an optimization problem here optimization problem with constraints. So let us, see what this method is all about? And we will generalize this idea. So let us say we want to minimize, let us say we want to, could be anything to maximize or minimize. And so, let us say to find out the stationary points of the function f to this f of x y, what we do is we do df, what is df in terms of, we can write it in terms of the partial derivatives dx plus partial f partial y dy and since we want to find out the stationary that means, locally the function does not change. So, that is the condition that we are looking for.

So, if dx and dy, let us say were independent. If they were independent, then will see, for this to satisfy what has to do is partial f partial x has to go to 0 and partial f partial y has to go to 0 individually. so that is the basic calculus, we understand that the first partial derivative should go to 0.

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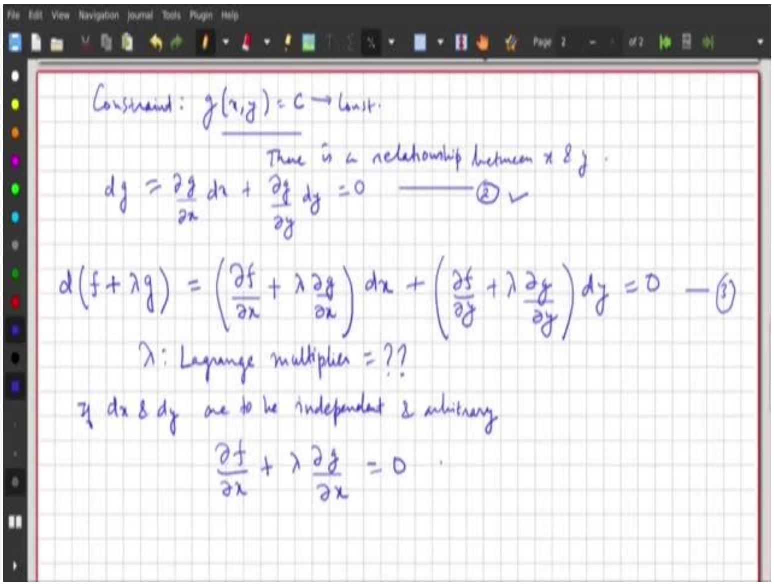

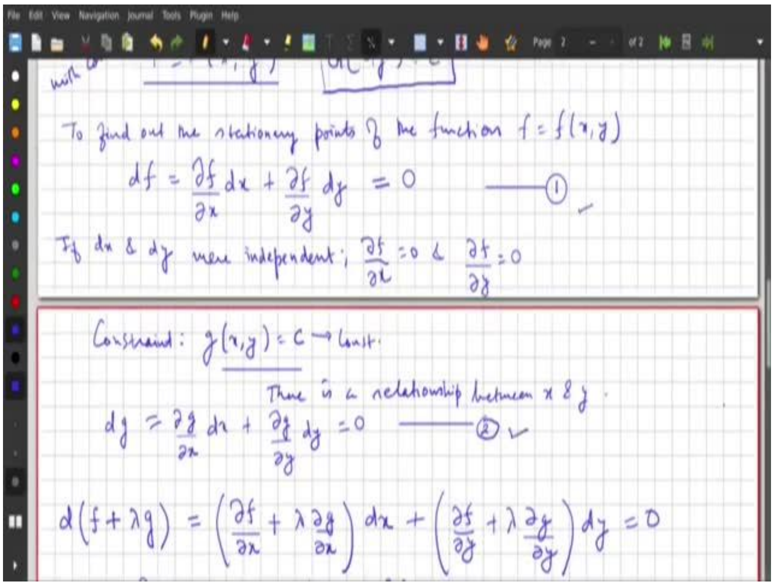

But now let us say we have a constraint. Say we have a constraint that is given by g of x comma y equals c. So, given this constraint, that means there is there is a relationship between x and y, so that is the, so that that means there is a definite relationship between x and y given the constraint and constraint given by g of x y equals c. So there is a relationship between x and y.

So if this needs to be satisfied, given that this is a constant, that means if we take a differential of g that has to go to 0, then what is the differential of g, we can write partial g partial x dx plus partial g partial y dy and that should go equal to 0. So now, let us say if we use, let us call this equation 1, and let us call this equation 2.

So, if we use equation 1 and 2, we can write it in this way, using an arbitrary we will see call lambda. So, what we can do is you can write it in this way d of f plus lambda g and that will become this will become df, which is given by partial f partial x plus lambda times partial g partial x dx plus partial f partial y plus lambda times partial g partial y dy and this is equal to 0. So, here lambda is called the Lagrange multiplier.

And remember that this is unknown this we do not know yet this needs to be figured out so, what that lambda is? But given equation 1 is true and equation 2 is true we can write in general expression like this for an arbitrary lambda which like we can write this condition for a particular lambda not arbitrary a particular lambda that satisfy this expression and we need to find out what that lambda is actually and that is the Lagrange multiplier by the way.

So, basically if you see that means if so, if dx and dy are to be independent and arbitrary, then for this equation for equation 3 to hold the coefficients of dx and dy themselves has to vanish. So, that means, partial f partial x plus lambda partial g partial x should go to 0.

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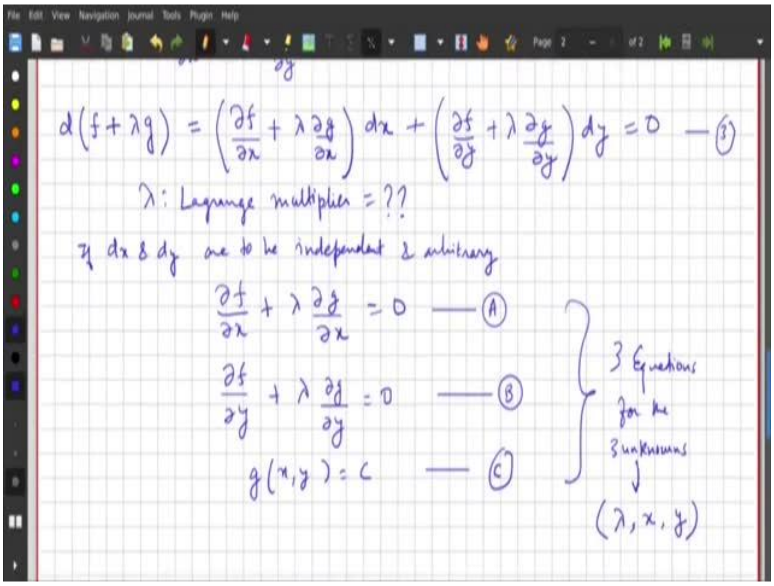

That is the equation called as A and partial f partial y plus lambda partial g partial y equals to 0, that is equation B. So given these two conditions needs to be true, for a particular lambda. So using equation A and equation B and using the constraint relationship, which is g of x comma y equals c.

Now, you see we have 3 equations. 3 equations for the three unknowns that we need to find out three unknowns. And what are those 3 unknown, the 3 unknowns are the lambda, the value of x and the value of y, where we want to find where the function is, at its extremum. So that is the general idea about how to find out, let us say, a function optimization problem given a particular constraint.

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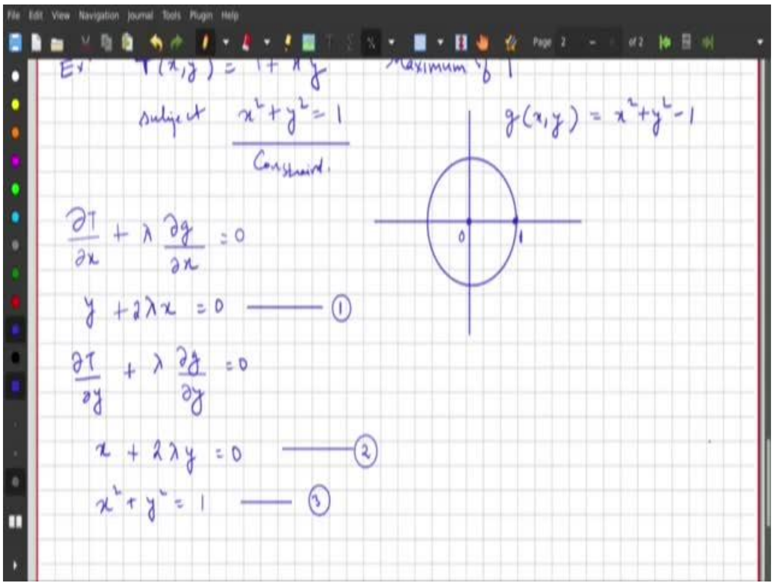

So let us do an example just to get this idea better. So let us say you have been given a function, T of x comma y equals 1 plus x, y. And we want to find out let us say, the maximum of T subject to the constraint subject to the constraint x square plus y square equals 1, that means we are not allowed to move outside the unit circle. So what we want to do is, we want to find out the maximum value of this function T, provided that x and y always stays on this circle. That circle is a specific set that is the unit circle, this is a circle of radius 1. That is a condition that we need to find out.

So let us see how to do this. So let us, what we will do is we will write the condition. So we have one constraint, this is the constraint equation. So we can write all these equations A, B, and C for the specific case. So that will become partial T partial x plus lambda times partial g, partial x equals 0 where, let us define g. What do you mean, it is a g of x comma y is basically x square plus y square minus 1, so that is the circle so, g equals 0 defines the unit circle that is the constraint.

So partials if you see from this equation, partial T partial x times y plus lambda and partial g partial x will become 2 x will come here, so we will have x equals 0, so let us call that equation 1. And similarly, we will have partial T partial y plus lambda partial g partial y equals 0. And if you see partial T partial y will become x will become x plus lambda and partial g partial y is twice, so there is two times y equals 0 that is equation number 2. And remember, we have the constraint equation itself, which is x square plus y square equals 1 so that is equation number 3.

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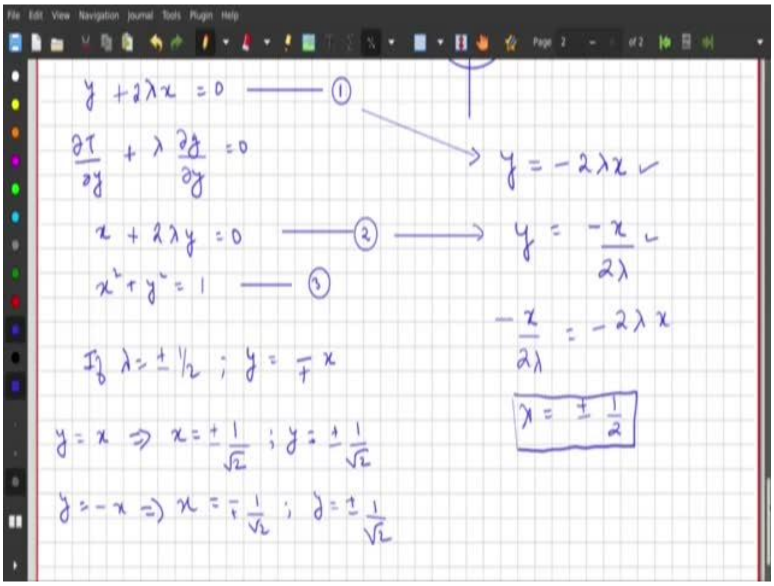

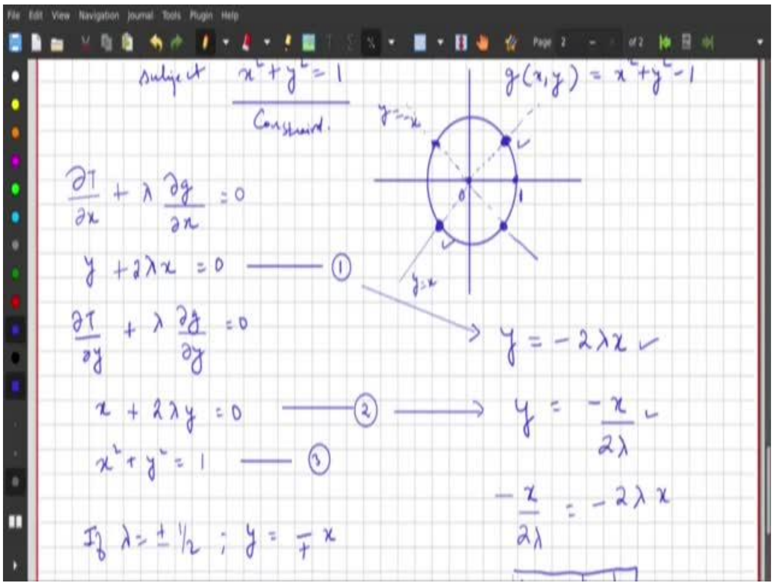

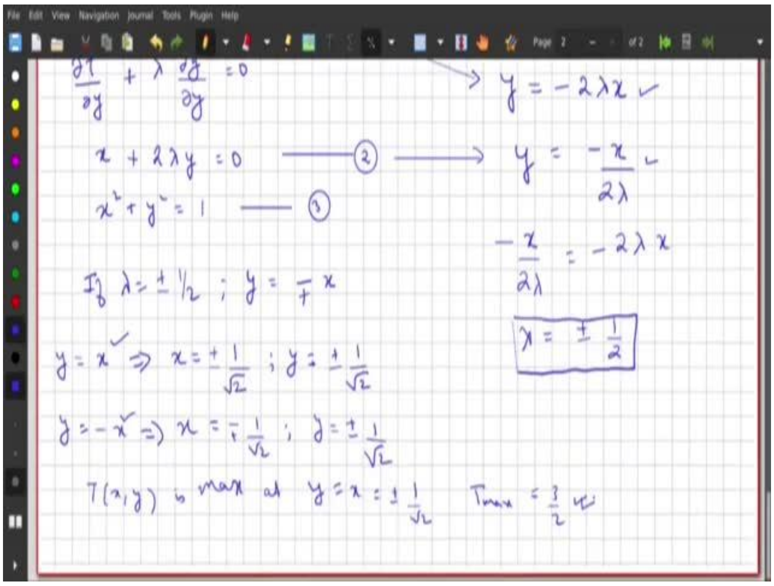

Using all these 3 equations, what we can find out is from equation 1, you can see from this equation you can see that we can write y equals minus 2 lambda x and from this equation, we can write y equals minus x plus 2 lambda and if we equate these two y, we can solve for lambda that will become minus x by 2 lambda equals minus 2 lambda x. So if you solve for lambda, we will get lambda equals plus or minus half. So if we figured out what lambda is? So if you see if lambda is plus or minus half and if you substitute it right here, what we will get is if lambda is plus or minus half, y is if lambda is plus half, so you will get y is minus x. and if lambda is minus, this will become plus.

So let us say we have y equals x so, that for the y equals x the critical points will become a given that we know x square plus y square equal 1. So, this will become x will become plus or minus 1 by root 2 and y will become plus or minus 1 over root 2. And similarly, for the condition y equals minus x will find out that x will become minus plus 1 over root 2, and y will become plus minus 1 over root 2.

So, we found out all the critical points with all the combinations with x y for plus minus 1 over root 2 and you see these, these two critical lines lie on y equals x and y equal to minus x, if you remember the diagram, so, that means, so, that is the 45 degree line y equals x this is y equals to x and similarly, this is another critical line y is equal to minus x.

So, wherever the extremum is happening, it will lie on either these two lines. So, these are the critical points that we found out plus or minus 1 over root 2 both in x and y. And now, if we just substitute the values of x and y, we will find out that T, the T of x y is max at y equals x equals plus or minus 1 over root 2 and the value of T max is 3 halves that means temporary or let us say T is maximum on these two points along this line, and specifically on these two points, and the maximum value of T is 3 halves. So that is an example of an optimization problem where we figured out we extremize the function T subject to a given constraint.

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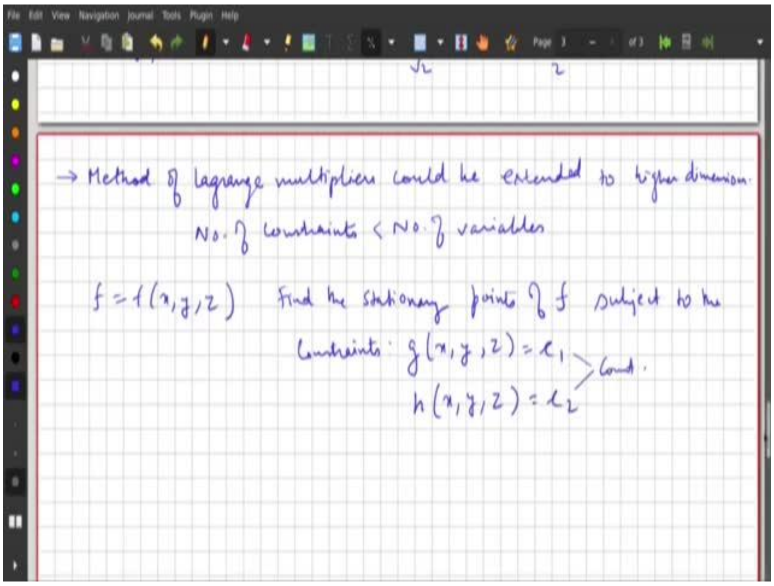

So, this idea could be explained to or could be extended to higher dimensions, higher dimensions where we have let us say a function of 3 variables. So, let us say the method of Lagrange multipliers could be extended to higher dimensions, higher dimensions, the only condition that we need to keep in mind is that the number of constraints should be less than the number of variables, the problem the independent variables differentiating with to prevent it from becoming over constrained problem.

So that is a general thing where it works. So let us say you want to find out the function f is equal to f of x plus comma y comma z you want to find out where when or where is, let us say suppose the problem like this, find the stationary points of f, subject to the constraint. Now, let us say we have g of x comma y comma z is equal to c 1 and we have another constraint h comma x comma y comma z is equal to c 2, where these two are constants. So, now we have two constraints.

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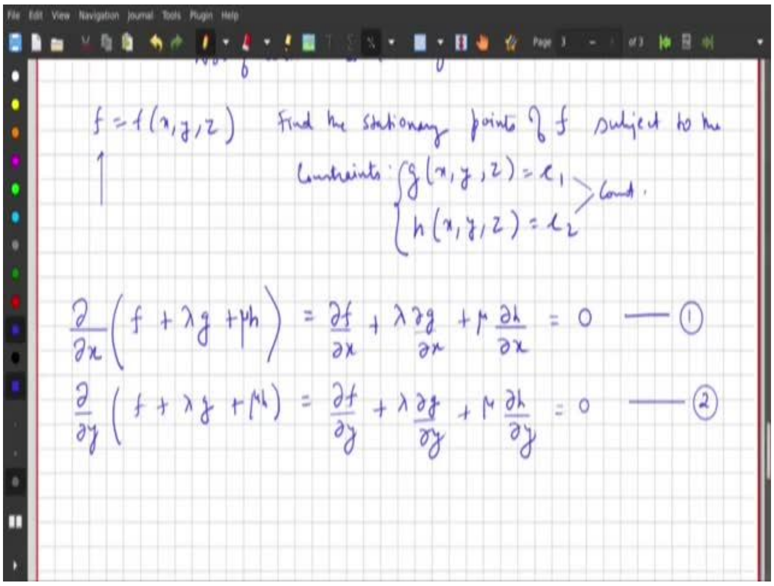

So, what we need to do is we need to find the stationary points of this function f subjected to these two constraints. And if we just extend our previous idea, the equations will become partial partial x (())(24:10) f plus lambda g plus mu h and then that will become partial f partial x plus lambda partial g partial x plus mu partial x partial h partial x equals 0. So, this is now equation 1.

Similarly, we can write expressions in the y in the z direction. So, this will become f plus lambda g plus mu h and this will become partial f partial y plus lambda partial g partial y plus mu partial h partial y and that is equal to 0 that is 2.

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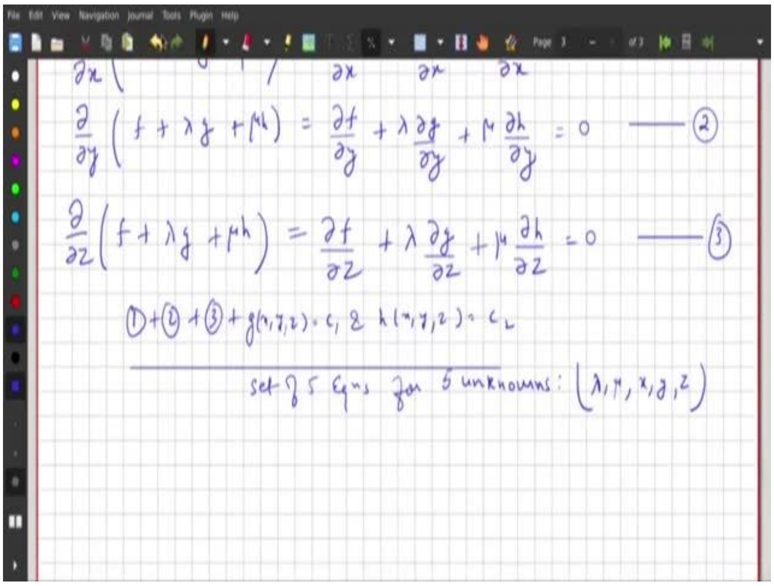

And similarly, the third dimension partial with respect to z f plus lambda g plus mu h equals partial f partial z plus lambda partial g partial z plus mu partial h partial z and that goes to equal to 0. So, these are the 3 equations that we got from the constraints. And using these three equations, so, question 1 plus 2 plus 3 plus the two constraint equation which we have g of x comma y comma z equals c 1 and h of x comma y comma z is equal to c 2 in we see, we have a set of a set of 5 equations that we need to solve for 5 unknowns, and what are the unknowns the unknowns are, you see lambda, mu, and the points where the function is stationary x y z.

So these forms a closed set of equations which where we can solve for lambda mu, x, y and z. So, that is the general idea of the method of Lagrange multipliers. So we saw an example where with one constraint, and we generalize the idea to any like a higher dimensional function of 3 variables with two constraints. So this could be generalized 3 dimensions, the only thing that needs to be kept in mind is the number of constraints should be less than the number of independent variables.

For example, here, there are three independent variables x, y, z, but we have only two constraints. So, if that thing is true. We can use the method of Lagrange multipliers to do our optimization problem. So that is for the segment. So we will see you in the next segment. So thank you for being there. And we will see you in the next segment.