Introductory Mathematical Methods for Biologists
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Lecture - 11
Curvature and Second Derivative

Hi, welcome to this lecture on mathematical methods for biologists. Today's topic is curvature and second derivatives. In this lecture, we will discuss basically what can derivatives tell us about up down curves. So, it is about curvature and second derivatives. So, so far we have been studying about first derivatives, which is essentially the slope and we briefly said that we know that slope m is; how does the function changes.

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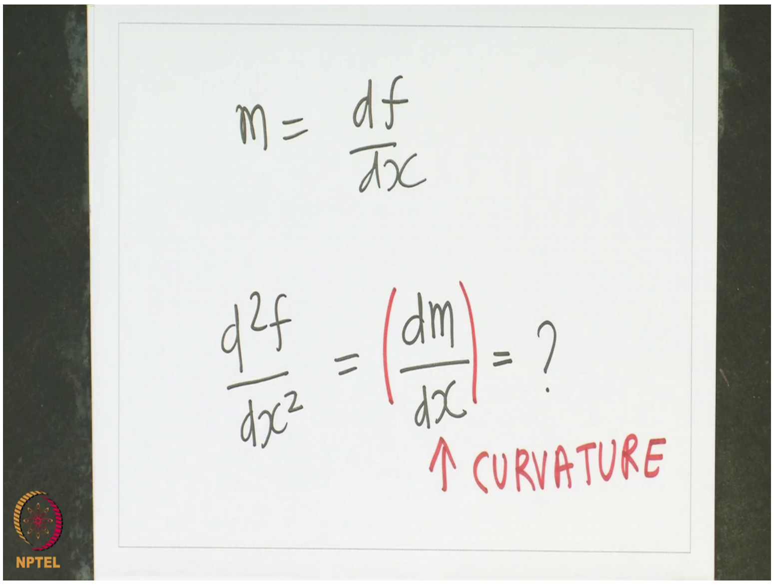

We also briefly said that the second derivative which is d square f by dx square, which is how does the slope itself change how does the m itself change, and we briefly told about it, but we will understand this in detail today. So, we will graphically and this think about the second derivatives and higher order derivatives if possible. So, first let us look at a curve anything that is turning. So, what is a curve?

Something that is turning this curve.

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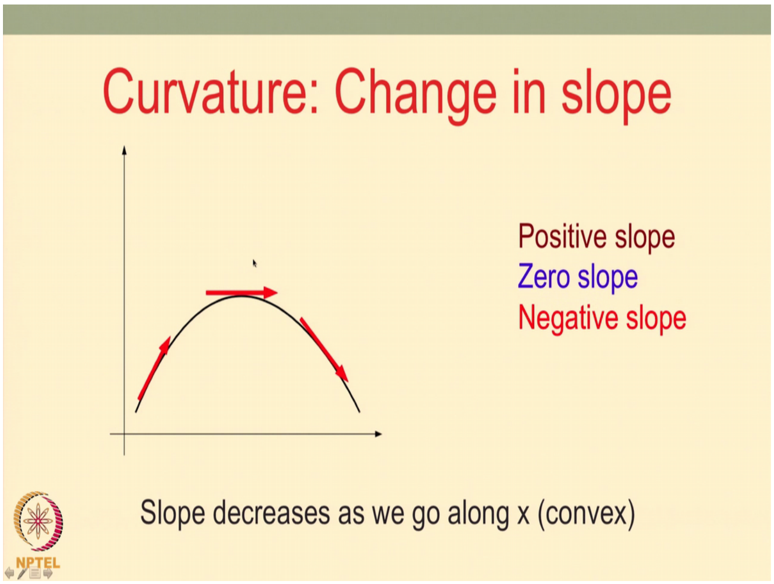

So, look at this curve. So, if we have this curve and if you think about the slope at different points. So, slope is if we take any point and draw a small straight line let us call it tangent. So, you take any point and draw a straight line tangent there. So, this is the slope here, if I take here this is the slope here the if you take the slope was here.

So, what we can see here is that in the left side here, the slope is positive that is the function is increasing as a x increases. But if I look at 2 points the slope itself one can see that the slope itself would decrease and here if I take the if I look at the peak this the tangent or the straight line if I draw a small straight line, for a small segment it will be essentially parallel to the x axis so; that means, the slope was nearly 0 there.

At this if I take an extremely small delta x 10 in to 0, I would get the slope to be 0. Then if I further come along the x somewhere here, if I take a point and draw a small line there a straight line there, that is a tangent I would get that the slope of that straight line would be a negative number. So, this is a negative slope. So, we had a positive slope which means the function increased as x increased, here locally if I take a small point the function kind of do not change function does not change much. So, the slope was nearly 0, and here the slope is negative; that means, the function is decreasing if I increase x.

So, the point is that in any curve the slope will change and this change in slope is defined as curvature. So, as we saw here d m by dx this thing dm by dx the change in slope is called curvature. So, this thing is called curvature, that is; how does the slope itself change dm by dx. What we know is that if I have a curve which is like shown in the slide, if I have an increasing function or a decreasing function.

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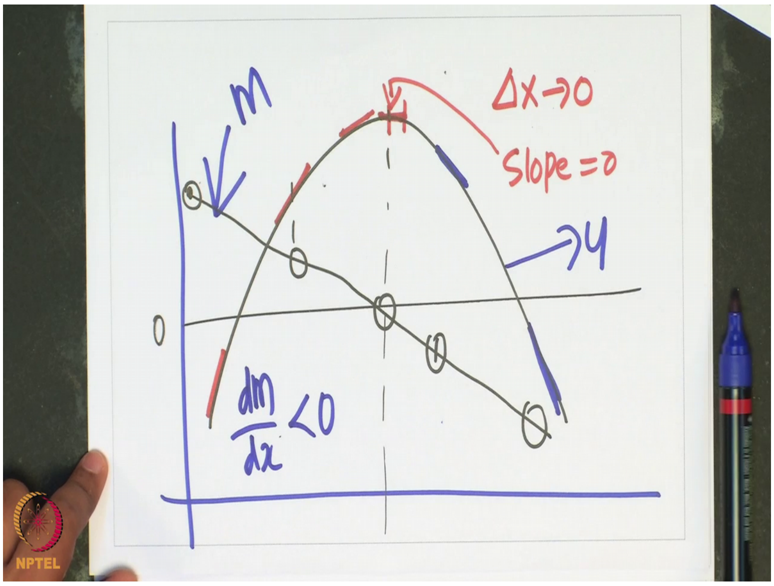

Here the slope will be positive it is a positive number, if I go here and draw a small line the slope is positive then it is a smaller value. So, this is a higher positive value if this is 10 this will be 6.

And if I further go down the slope has further reduced, and exactly at the peak if I take a very small extremely small delta x in the limit delta x going to very small, it will be essentially like a horizontal segment; that means, the slope there will be 0, the slope will be 0 right at this peak. And if I further down here you will have a negative slope, if I just come down further here, here I have a negative slope and if I come here further I have a negative slope again. But this negative slope is the small negative number and this is a larger negative number. So, I will have a slope starting from a high positive number coming down to 0 and increasing to a larger negative number.

So, that is what the slope of this curve would look like. So, if I plot if I were to plot the slope of this for accordingly here I will have a large positive number. So, I will have a large positive number, here I will have 0. So, let us let me call this 0 let us if I just define this as my 0. So, I have a large positive number somehow decreasing, I do not how is as it will decrease it depends on whether is a quadratic curve about what curve it is, but somehow is decreasing and then becoming negative and larger and larger negative. So, depending on the precise nature that is a quadratic curve will be precisely a straight line otherwise this will have some function.

But we do not know whether it is a straight line or what, but nonetheless we know this much that here the slope is positive, here also is positive but a smaller value, here it is 0, here it is an small negative here it is further down smaller negative. So, we know this and we can get this slope itself. So, the point here is that the function here if you look at it, the change in slope is call the curvature the slope decreases as we go along the x such curves are called convex and the m which is dy by dx and the dm by dx which is the change in slope is called the curvature and here d by dx of dy by dx, it is mathematically written as d square y by dx square.

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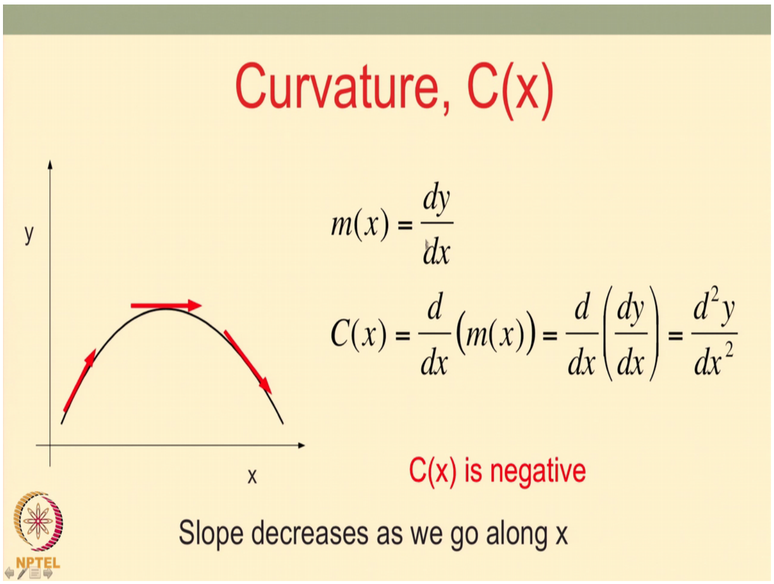

Which is the second derivative if you compute for this the c of x this will be negative, is what I am trying to say is that if you look at here, this is this if this curve one is our function y. So, this is our function y, this is our function m slope. Now if you look at how does the slope itself changes, if you look at dm by dx the slope how does the m with x by x changes this dm by dx is negative you would see that dm by dx is negative its a negative so; that means, this here the curvature is negative. So, the C of x the curvature is negative.

So, the slope decreases as we go along the x therefore its second derivative for such a upside down curve, which is called a convex curve. If you have an upside down curve like this this will have a negative slope and therefore, d m by d x which is C the curvature is negative. Curvature is the slope of this straight m curve right. So, now, let us look at the curve which is like u like.

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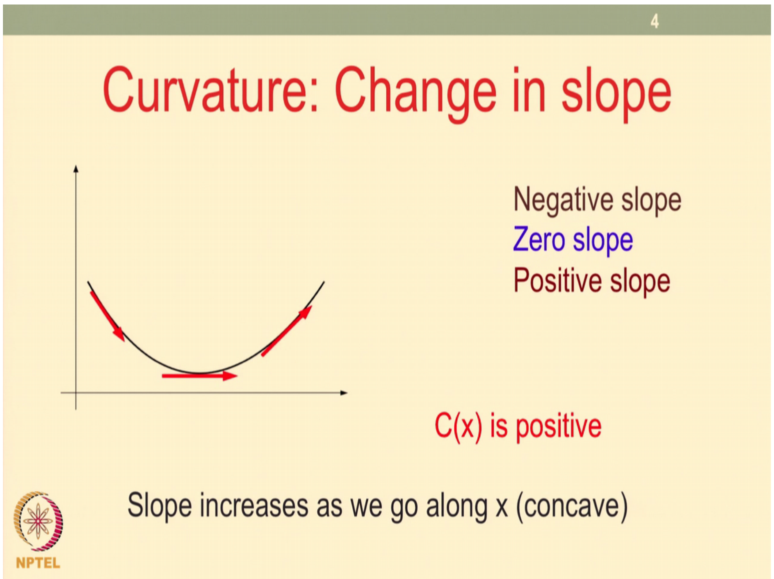

So, if you take such a curve at the beginning for small x values, if I draw a small tangent the slope is negative. Here at these minima the slope is very small that is near 0 and here the slope is positive. So, the slope increases from a negative value to 0 and to a positive value as we go around the x and therefore, the change in slope here is positive.

Therefore C of x which is a curvature which is positive, we can draw exactly same as we did earlier we could draw a curve.

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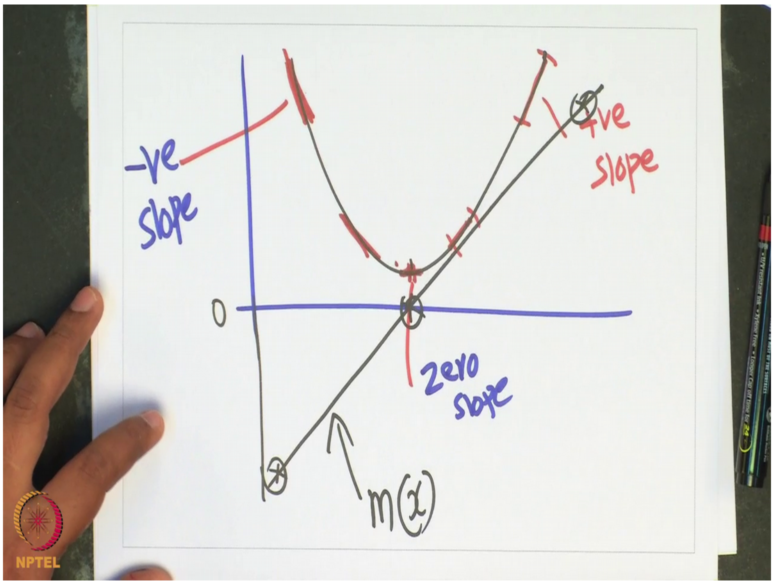

Which is like this and we look at the slope at different points, here if we look at the slope which will be a negative number. Here is also a negative number, but this is more tilted than this. So, this is a larger negative number the slope here will be larger compared to the slope here. Here if I take a very small delta x locally the slope will be 0. So, here this is negative slope. So, let me write here negative slope zero slope locally, here if I look locally its a positive slope.

If I look here it is also a positive slope, but this is tilted more. So, compared to this this is more tilted. So, this is more positive. So, this is positive slope. So, the slope change as we go along the x the slope changed from a negative number to a positive number. So, if I extend this below and consider this as 0 here the slope was negative some negative number, here the slope was 0 and here the slope was positive. So, the slope if I plot it would look something like this. Depending on the precise nature of the curve the slope could differ, but this is my m of x curve the slope curve. The slope itself increase with x that is the idea here that the curvature which is nothing, but the measure of change in slope it is a measure of how the slope changes the slope was changing from negative to positive therefore, the Cof x is positive slope increases as we go along the x curve.

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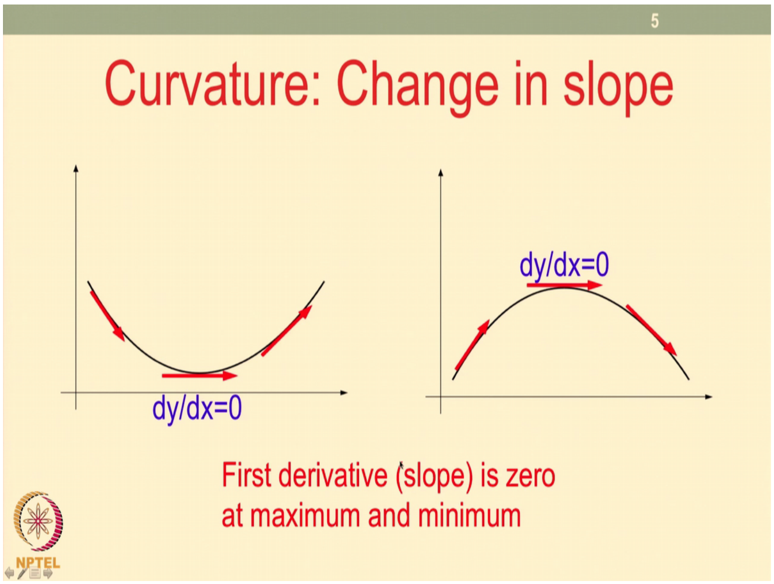

So, the curvature is nothing, but change in slope and the first derivative which is a slope of 0 at maximum and at minimum and you have these 2 curves which is like u like curve and this is upside down curve and this will have. So, here which is like a u like has a positive curvature. So, this is has a positive curvature while this has a negative curvature. So, this is the thing that we should understand, the second derivative whether it is positive or negative if the second derivative is positive you will have one kind of curve if second derivative is negative you will have another kind of curve.

So, this is always important to remember in this case second derivative is as a different sign from the second derivative in this case. And there are many curve functions which we are very familiar for example; if you take energy of a spring like protein like energy can be written as x.

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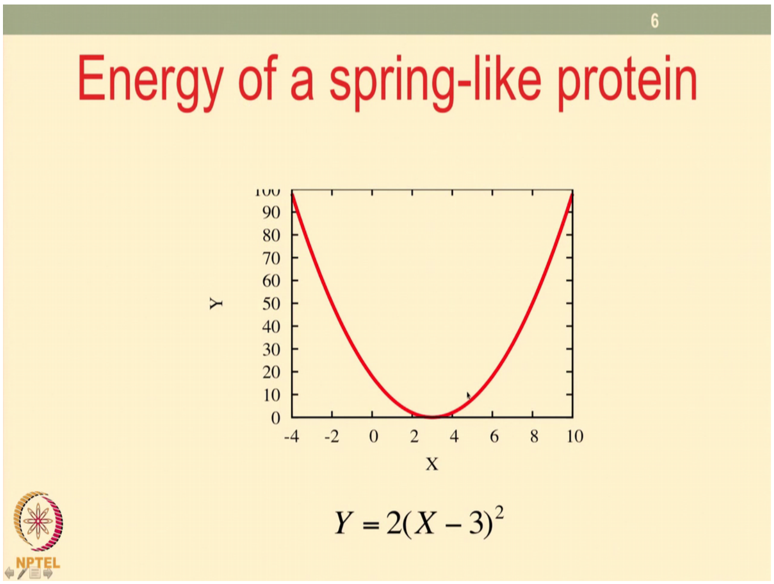

Minus x 0 whole square like half kx square is typically energy of a protein like curve, a protein like spring like protein if you like an energy function which could be a quadratic function like this for example.

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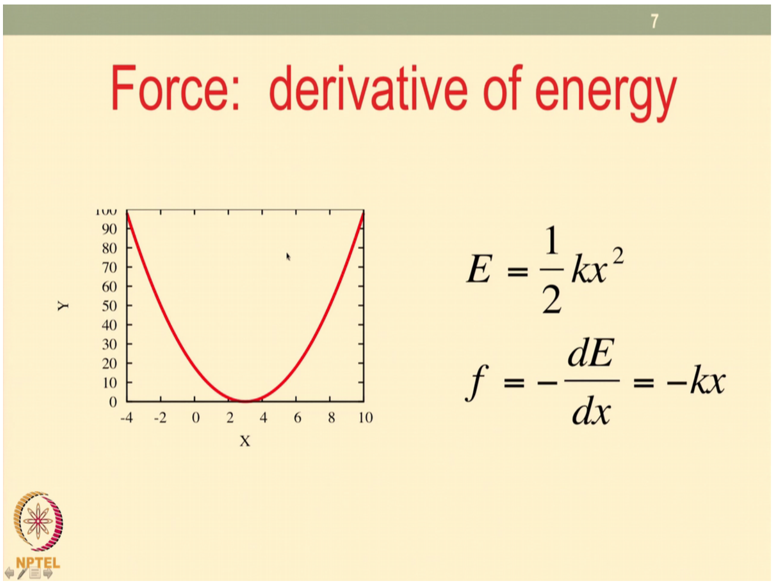

E is equal to half kx square or k x where x minus x 0 whole square if you wish it will be a quadratic function you required function.

The force will be a derivative of this energy, we know that force is the derivative of energy if you go de by dx and you have a negative sign that is a force, and force will be a linear function with respect to x and therefore, we can compute the force.

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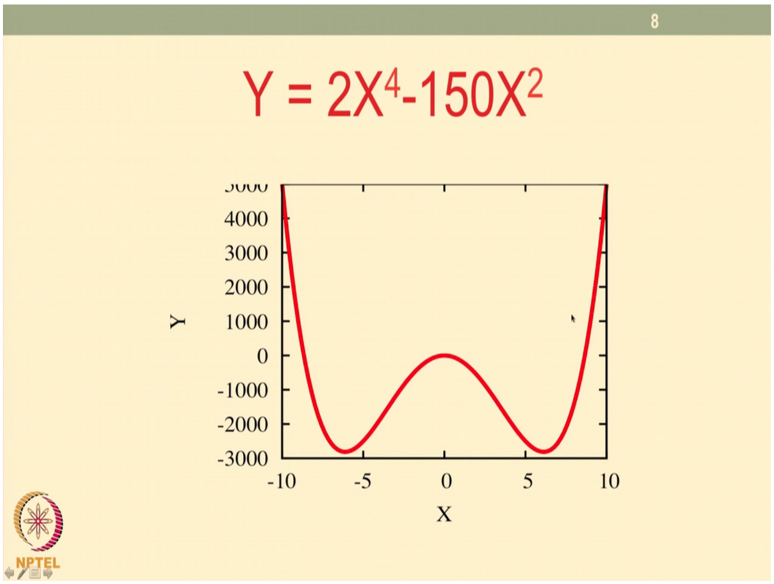

We also would have a seen curve with free energy and functions like this which has maxima and minima; there is a maxima here and 2 minima here. So, we would have seen many functions which has maxima minima and all that and we will come across and discuss them in detail many a function, but as we get familiar ourselves with functions what the thing that we should learn is that.

Any function that you plot right any function if you think about draw any function that you like right if you ask if we ask you to draw.

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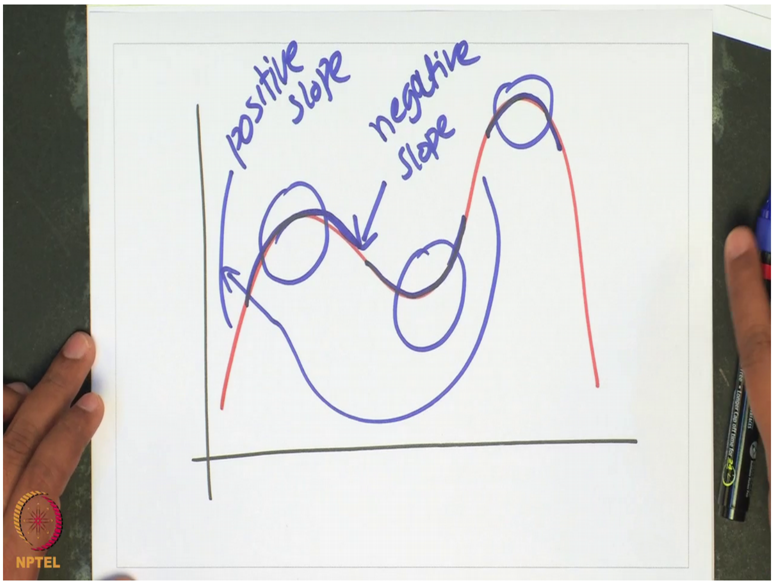

Any function a randomly random smooth function if you asked to draw; typically you would draw something like this. Whatever it could be any function, what it has any curve you draw will have is there will be some maximum, there will be some minimum and there will be like some positive and negative slope. So, here there is a positive slope right positive slope regions, there will be some negative slope regions. So, this is a negative slope region, this is a positive slope region this is like.

A positive slope region this is a negative slope region and this is maximum. So, if you draw any curve that you wish a smooth curve, typically what it will have is some positive slope regions, some negative slope regions, some positive slope regions here some negative slope regions, some maxima 1 or 2 or many, some minimum or minima could be one too many depending on the curve you draw, but you can for simplicity you can decompose any curve imagining it as some things like this. So, if we understand which region is the positive slope with region as negative slope which region has curvature which is positive curvature or negative curvature?

So, this is like inverted u, and this part is like a u right this part is like an inverted u if you wish and this is almost like a u right. So, we just learned that one of this region has a negative curvature while this has a positive curvature. So, some religion with positive curvature, some region with negative curvature, some region with positive slope some region with negative slope. So, any curve any smooth curve that you wish any data that you would get, essentially we will have some region with positive slopes some region with negative slopes some regions with positive curvatures some regions with negative curvatures.

If we understand this that would simplify any curve a lot; and by understanding its slopes and curvatures we can draw reconstructs curves much easier. So, what we will learn in the coming classes coming later is how to reconstruct the curve if we only know about the slopes and its derivative right. So, if I just tell you some information, that you have a curve which has no curvature only positive slope right. If I just tell you that you have a curve, you have a curve which has which has no curvature let me write again no curvature only a positive slope.

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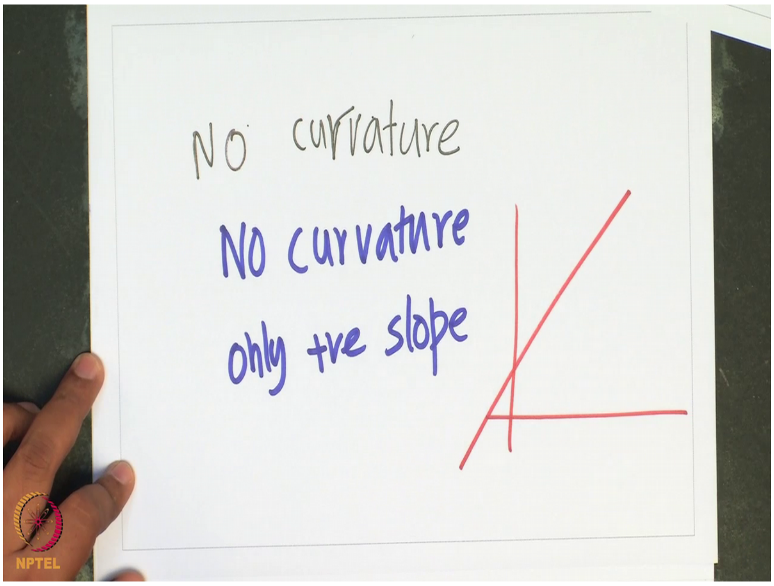

If this is the instruction given to you immediately you know that the function has to be a straight line because this is the only positive slope and it has no curvature. If we tell you that the function has if we said it has positive.

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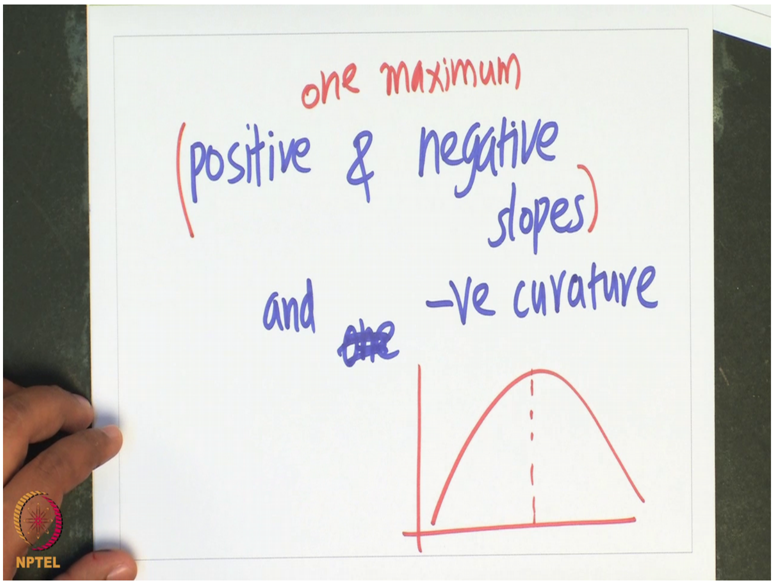

And negative slopes and one negative curvature and there is some region I would not say one and there is some region with negative curvature. What would it mean negative curvature we immediately know that negative curvature would mean like this right? So, it has to look like this, it as a positive slope negative slope and the curvature is negative. You could also say that it has 1 maximum or a minimum.

Like if this is a maximum. So, if I say it is positive and negative slopes and one maximum if I say one maximum it would surely have a positive a negative slope and it has a negative curvature. This I could instead of this, I could say one maxima or maximum and then a negative curvature if I tell you this much you should be able to guess that the function would look like this because roughly like this because this is the only possibility. So, if I if you want to under similarly if I say it has one minima or minimum which would mean this is a positive curvature, this would also you would know that the curve would look like the opposite and.

So, if one could give informations like this. So, instead of giving you the data of the function itself, instead of giving you an f of x itself you could give we could have information about the slopes, we could have information about the curvature and that is also an equal and equally valid and sufficient information sometimes to draw and understand the curves in understand the functions. So, we would understand the function f of x, we would also equally understand the derivatives df by dx, d square f by dx square all of this convey information. Just like saying f of x would look like this equivalently we could all say there is the slope looks like this, the curvatures looks like this therefore, the function has to look like this. So, the whole of mathematics calculus is understanding this play between function and its derivatives.

And pretty much everything in nature lot of things in nature is also about understanding this understanding this in relation between function and its derivatives. Just like we saw energy and force are function and its derivatives, there are many things in nature we would see that concentration and the flow has a relation between function and its derivatives right. So, there are many other things that we would see in nature, which has one of it is a function the other one is derivative. And there is also second derivatives; curvature is something which is very common throughout the nature for example, if we take a cable which is a curved which is a curve.

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So, this is instead of it is straight this is curved and there are many filaments in biology which is like a roughly like a cable like even DNA is like a filament, and there are many bio filaments. So, if we take this cable, and if we want to describe this the shape of this right. One of the major challenges in biology is to describe shape of molecules how? How the molecules are, what is the shape of a molecule. So, if I want if you to the describe a curved molecule and mathematically we have to use this idea of curvature positive slopes and negative slopes.

So, if we want to say that my bio filament has this particular shape, we would surely want to know it has a particular curvature. Not just that you would want to ask a question if I have a bio filament and it is getting curved it is forcefully some enzyme some machinery against the cell is bending it and curving it there is all of DNA bending proteins. So, how much energy would it cost to bend a filament how much energy would it cost to bend and make a curvature on a DNA. So, if you want to understand and if you want to think about in mathematically, we would want to write equations for the curvature because the energy would depend on whether it is curved a little bit whether it is curved a lot.

So, if I want to take any curve and bend a little bit I want on only a little bit of energy, but if I want to bend a lot, I will need a lot of energy. So, the energy to bend the curve would depend on how much it is curved. So, this is common sense. So, based on that let us write here. So, this is something that we would want to use.

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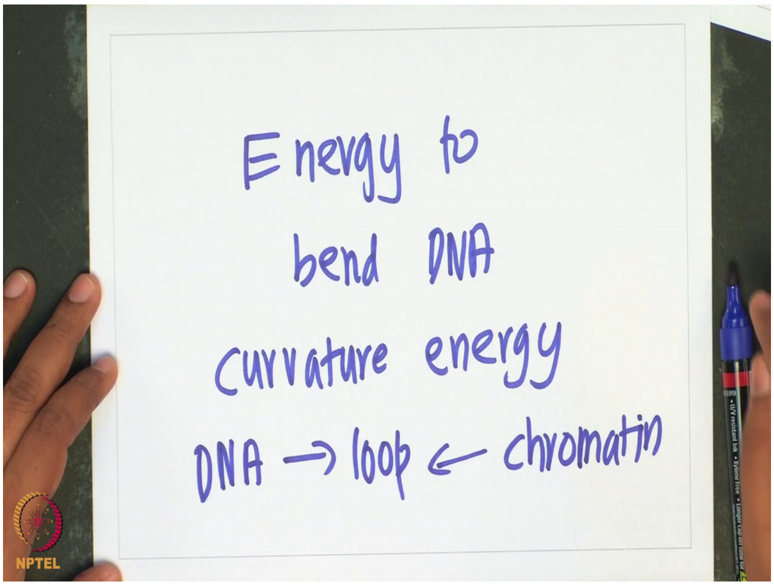

Energy to bend DNA right energy to bend DNA. So, this is called curvature energy how much energy is needed to curve, how much energy a protein must be spending to curve a DNA; DNA can it is well known that DNA forms loops and d when the DNA is coiled to chromatin the DNA is looped.

And many processes in biology DNA has to loop right. So, you would know that chromatin is DNA package and the loop ring of DNA curving of DNA. So, if you want to understand this quantitatively, if we want to use scientific language to understand chromatin for example, we would need to understand the mathematic you need mathematically described curvature. It is not just chromatin alone like the cell itself the membrane itself is curved. So, the curvature of the membrane right how protein would bind in a curved membrane surface right vesicles which are curved structures. So, the curvature is all our by is this all our in biology right.

So, if you want to understand curvature you want to understand how much or anything that we see, how much is it curved is it curved a little bit or is it curved a lot to know that the what we would calculating is to calculate the second derivative.

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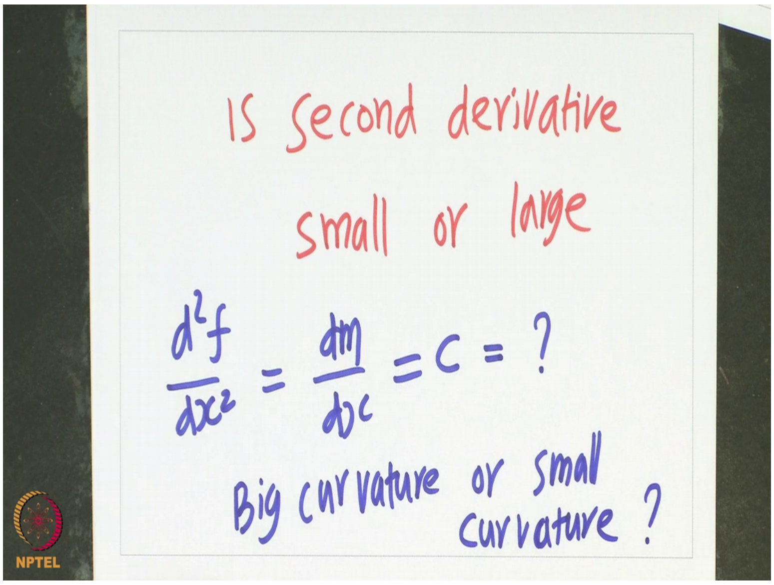

So, is a second derivative small or large, that is if I calculate d square f by dx square which is same as dm by dx which we call as C. Is this big or small this would tell us you tell you that it is curved little bit big curvature or a small curvature. This is something which we want to know very often in biology and mathematics using the language of mathematics we would learn this curvature and how to compute this. So, we would now go ahead and learn how to compute the curvature. So, to summarize this lecture basically what we described is all about second derivatives we just said that.

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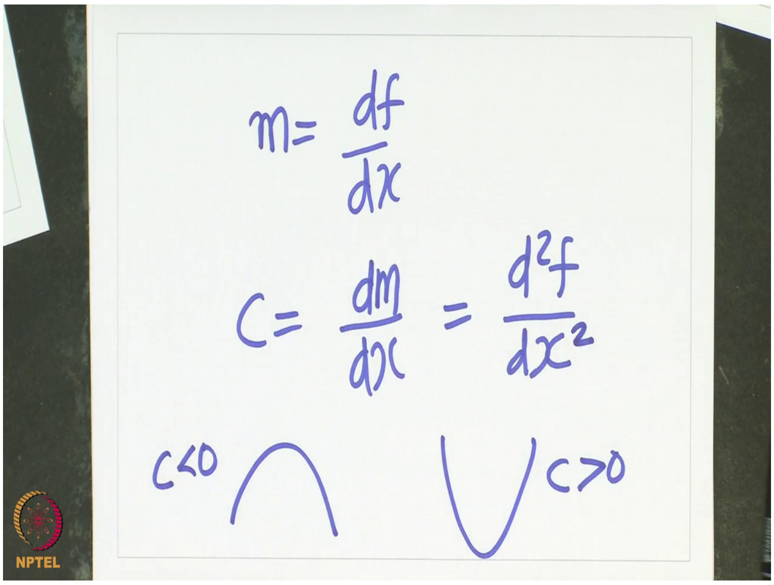

M is the slope and curvature is dm by dx how does the slope itself changes and which is the second derivative of the function and there are curves like this. So, C is dm by dx which is d square f by dx square.

So, when you have 2 kinds of curves, C is less than 0 and C is greater than 0 you have curve which is upside down like this and u like. U like will have curvature greater than 0 positive curvature and negative curvature. So, this is the summary of what we learned so far with this we will stop todays lecture and continue to learn in the coming lectures.