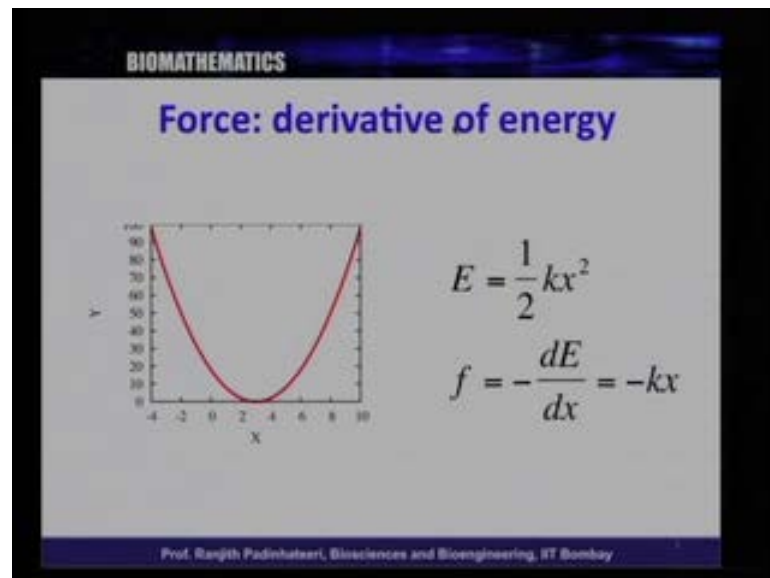


**Biomathematics**  
**Dr.Ranjith Padinhateeri**  
**Department of Biotechnology**  
**Indian Institute of Technology, Bombay**

**Lecture No. # 09**  
**Differentiation and its applications (Contd...)**

Hello. Welcome to this lecture on Biomathematics. In this lecture, we will continue discussing some more applications of differentiation and how we can learn, whatever we plot, we learnt so far; how we can use the things that we learnt so far, to sketch some of the functions, to plot some functions using pen and paper, using hand, how do we sketch some functions from the knowledge we gained so far; the knowledge of the, using the, using the things that we learnt from calculus, so, so far, we will discuss, how to plot some functions. Before that, we will continue, we will discuss some of the applications of derivatives. So, we discussed some example applications. We will discuss more Biological examples, some more examples in Biology and then we will go ahead.

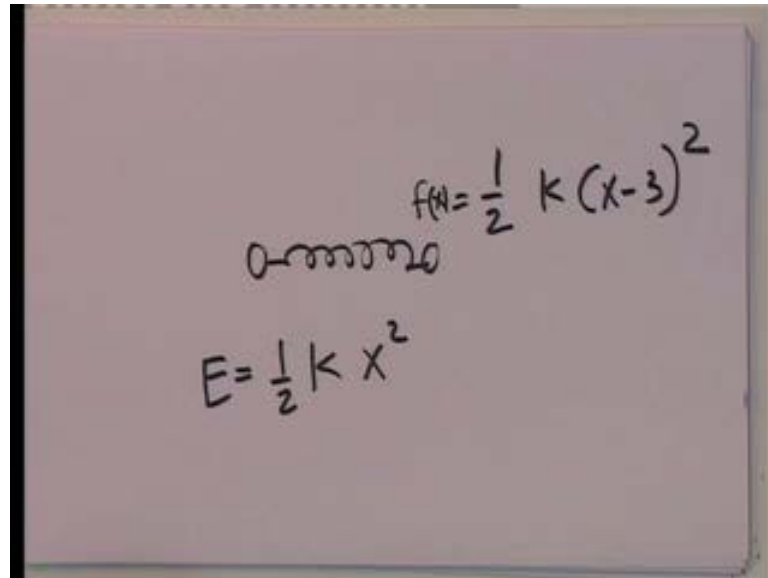
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So, the lecture is again, name is Differentiation and its applications. And, the simplest...So, as you know, we have been discussing the, we have discussing, we have discussing, derivative, the idea of differentiation and the, as the part of the calculus. And,

when you say derivative, this, one of the thing that will be very useful, is to know that, force is a derivative of a energy. So, let us have a look at the slide here. The title of the slide is force as a derivative of energy. So, now, when I say force is a derivative of energy, let us consider a spring like protein. So, a protein that can be stressed a bit.

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So, if you, if you draw here, you have a, you have a spring like protein, a protein that, something like, which can be stressed. So, you, you can apply some force on it and then, stretch it. So, you have this energy, so... We know that, the energy of such stretching energy is  $k x$  square, half  $k x$  square - this is the energy. We know that, the energy of a spring or anything like a spring, anything stretching energy, the elastic energy for stretching, is half  $k x$  square. So, that is what written here,  $E$  is equal to half  $k x$  square. Now, if you know this energy, then, finding the derivative of this,  $d E$  by  $d X$  with a minus sign will give you force, in this case. So, let us calculate the  $d E$  by  $d X$  of half  $k x$  square.

So, we have, what is shown here is the, is the plot of half  $k x$  square. So, this is basically, some, this is not exactly half  $k x$  square; this is half  $k$  into  $x$  minus 3 whole square; something we discussed in the last class, half  $k$  into  $x$  minus 3 whole square. We discussed this function in the last class and this is what is plotted here. And, that means, it has a minimum at  $x$  equal to 3 and so on. So, both this functions  $k x$  square and  $k$  into

x minus 3 whole square, if you find the derivative, you will get some function, which looks like k times x. So, let us see first, **first**, what is the derivative of half k x square.

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$$\begin{aligned} E &= \frac{1}{2} k x^2 \\ -\frac{dE}{dx} &= \frac{1}{2} \frac{d}{dx} [k x^2] \\ &= \frac{1}{2} k \frac{d}{dx} x^2 \\ &= \frac{1}{2} k \cdot 2x = \underline{-kx} \end{aligned}$$

So, let us look at E is equal to half k x square. d E by d x is half times d by d, half is the constant. So, we can take it outside; k is also a constant. So, you can also, take k also outside. So, is basically, k by 2 into d by d x of x square. So, it is basically, d by d x of x square is 2 x. So, k by 2. So, you know that, x power n has n x power n minus 1. So, it is basically, k by 2 into 2 x, which is k x. So, this is the derivative half k x square, which is k x. Now, if you had a minus sign here, you can add a minus sign here, everywhere a minus sign. So, the answer also will have a minus sign. So, that is minus k x. So, we all know that, the force to pull a spring is minus k x; but k x, the minus sign only indicates the slope or the, there is a reduction of the force, which is toward the center; so, restoring force minus sign. So, essentially, half is equal to f half k x square has a derivative, **derivative** of this potential energy is force.

So, this is one thing where you always would need in Biology to calculate forces, because...You know, different kinds of potential energies like, there is electrostatic potential, there is elastic potential. So, all these potential energies, if you find the derivative of these energies, you will find basically, forces. So, and forces is the useful thing, which you can measure and which is important. So, any two charge, for example, when they move together, let us say, you have a positive charge and a negative charge,

when they attract each other, actually, one charge is attracting the other one and pulling them together, the force with which they attract is basically, the derivative of energy. So, the force and the energy are derivatives, which are very useful quantities, which we might need to compute. So, this is one application of differentiation. So, again, how do we use this idea of force in Biology?

So, there are very interesting experiments, especially like, in this era, where you have very fancy tools to do experiments and single molecules even. And, using these experiments where we can measure force and gather some information about the Bio-molecules. So, we will discuss now an example, where you apply force on a Bio-molecule and you measure the, measure something related to force and gather some information about the Bio-molecules, about energy and force.

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**BIOMATHEMATICS**

### DNA unzipping by force

$d$

$f$

$G(f)$  : Gibb's free energy

If we know Gibb's free energy we can predict distance, vs force relation

$$d = \frac{dG(f)}{df}$$

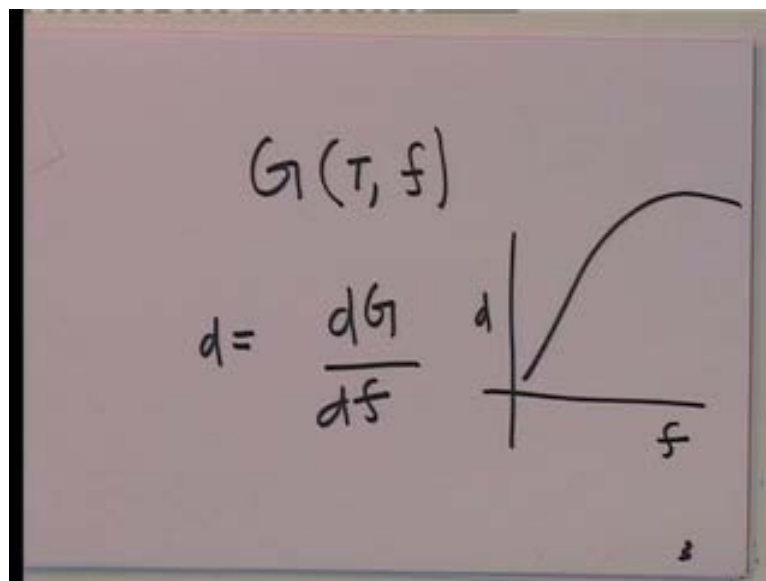
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So, let us look at the next slide. So, what you see on the left side is a schematic, tool like diagram, where we have a DNA. So, this is a sketch for a DNA, the red one. So, you have DNA, which ((obviously)) G T C, all this base pairs connected here. And, this is, base pairing broken here. So, this is one strand and this is the another strand. And, imagine that, one strand of the DNA is connected to a fixed glass plate or something; this is like a glass plate. So, you can attach one end of the DNA to a glass plate using some chemical, even using various way, there are the different ways, we, using which we can attach an end of a DNA to a glass plate. And, you can apply a force at the other end of

the DNA. One, single one of this strand you can hold, and apply a force. There are different mechanisms by which you can apply a force. They are called magnetic tweezers or optical tweezers or even, (( )) can apply some force on a DNA. There are different equipments available now, using which you can apply force.

So, imagine such an experiment, (( )); an experimental set up, where one end of the DNA strand is held at a fixed position, attached to a glass plate and the other end, is being pulled. So, we attach one end and the other end is pulled, so that, the DNA is zipping apart, unzipping. So, these are called DNA unzipping experiments. So, you might have, it is, you might know that, if you increase the temperature, the DNA will melt; the base pairs will break. And then, they will unzip and become two strands; you can separate this two strands. Instead of temperature, you can also use force, which is another thermodynamic variable. Just like temperature, force is a variable and you can apply a force and you can measure the distance. In Thermodynamics, there is a quantity called free energy, with which you, most of you are familiar.

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So, there is a quantity called Gibb's free energy, which is often denoted by  $G$ . This Gibb's free energy is a function of temperature and is a function of the force or the pressure. So, here is the force. So, you can measure the Gibb's free energy and the value of the Gibb's free energy depends on, how much temperature, what is the temperature of the system and what is the force you apply. So, this, in this case, the case of unzipping,

applying a force, you fix the temperature to, let us say, 300 Kelvin, or 310 Kelvin, whatever you wish, you fix the temperature, fix the constant. Then you vary the force and then, the, you can get the Gibb's free energy,  $G$  of  $f$ . So, once you know the Gibb's free energy, the relation between the Gibb's free...So, you can apply a force and measure this distance. So, this  $d$  is the distance from one end of the strand to the other end, where you are applying a force. So, this distance is  $d$ .

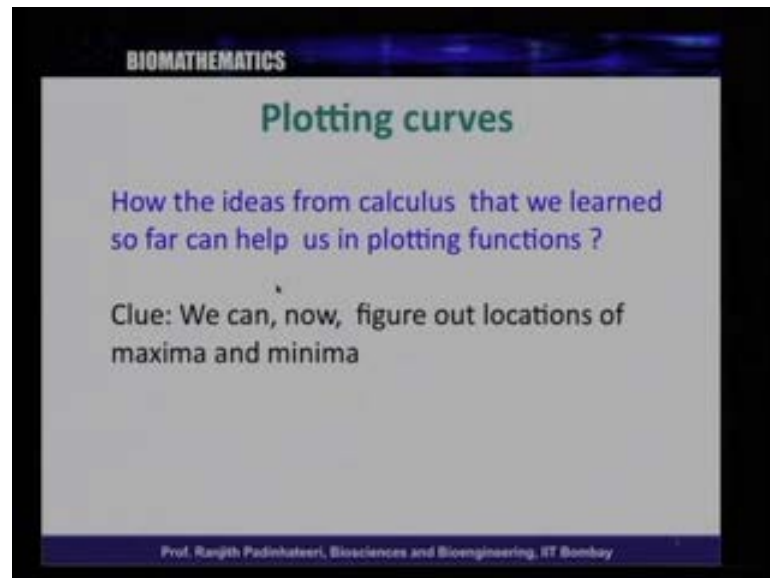
So, if you know the Gibb's free energy, we can predict the distance versus force relation by this particular relation. So, what I wanted to say here is that, the free energy and the force and distance are related in such a way that, through a, through a derivative. So, what is written here is that, if you know the  $G$ , the distance  $d$  is given by  $dG$  by  $df$ , given that the temperature is a constant. So, here, the  $d$  is the distance. As you see, in this picture here,  $d$  is the distance. This is the distance  $d$ . And, the more the force, the more the distance, in this case. But, using this relation, one can get even like a plot, versus, the force versus distance.

You can make a force versus distance curve. So, let us say, it could, it could look something like this; we do not know. Depending on the experimental condition, experimental system, the plot could look in different ways. But, this plot can convey lot of information. For example, let us say, about the strength; some of the base pair is very strong like, then, you, **you** need more force to unzip it. So, some of them are like, not so strong, then, they can come off very easily.

So, depending on the nature of base pairing, depending on their G C or A T, you would have different forces to unzip them. Let us say, all of them are A T, the force could be different and all of them are G C, the force could be different. So, one could, by this, getting the plot versus,  $d$  of,  $d$  versus  $f$ , you can imagine; then, one could get some idea about the content of the DNA and also, one can get some idea about the force needed to unzip it. So, just like melting temperature will give you some information about the DNA, the DNA base pairing, we can also imagine that, this kind of experiments can also give some information over the DNA structure. So, this is some experiment which is used very... It is a very, it is like a experiment that has been, the people have been doing this recently; like, post 90s and like, early in 2000s, like, last 20 years, trying to do this kind of experiments and they use this kind of relation, where free energy is related to the force and distance in such a way that, the distance is derivative  $dG$  by  $df$ .

So, this is the idea. So, here is another example, where you know free energy and the derivative is being used, using which, you can learn something about the system. So, that is the basic thing that I wanted to convey you through this. So, now, we will go to the second, that the part we are, I was talking about, where using the idea of, idea we learnt so far, how do we plot some functions.

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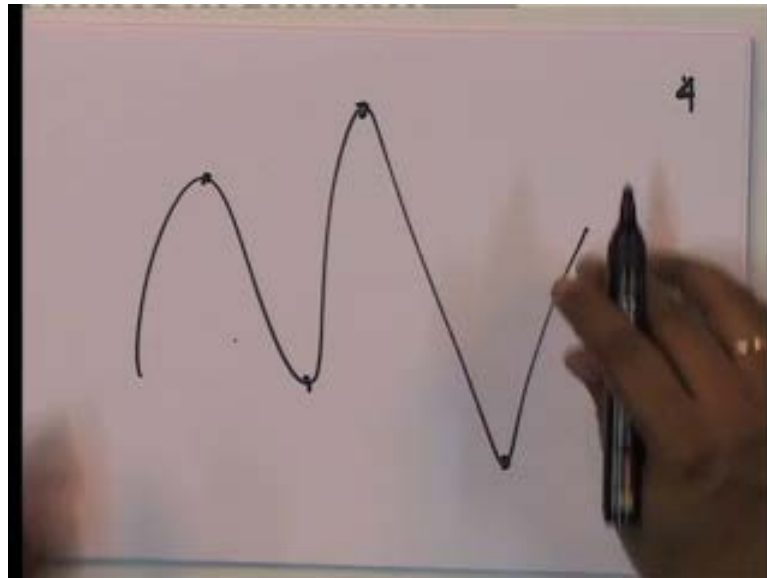


So, let us look at the slide here. So, the theme here is plotting curves and the question is, how the ideas from calculus that we learnt so far, can help us in plotting functions. So, we want to plot any functions using pen and paper. We want to quickly figure out, if you, somebody says, you,  $x^2$ ,  $x^3 - 3x$  or any function like,  $2x^2 - 23x$  or even  $e^x - x$ ,  $\sin x$ , any of this function, how does, how does this function look like; without figuring out each point by point, can we schematically plot this function? We can. You do not need to figure out...So...So far, what a computer or what the way you know it, as of now is that, any function you know, let us say,  $x^2$ , you calculate the square for each point, take  $x$  is equal to 0, calculate square,  $x$  equal to 1, calculate square,  $x$  equal to 2, calculate square...

So, that is the way we used to calculate. But, we do not need to calculate, for complicated function, we can very, you can easily plot it; you can schematically, you can roughly know, how would have, how will the function look like, by knowing some ideas that we learnt so far. And, what are the ideas? The idea we learnt last few lectures, for

example, we learnt about maxima and minima. So, the clue which I wrote here is that, we can now figure out locations of maxima and minima of any function. We can know that, where the function has maxima and minima. So, what does it mean to say, that a function has maxima and minima? So, let us think about it.

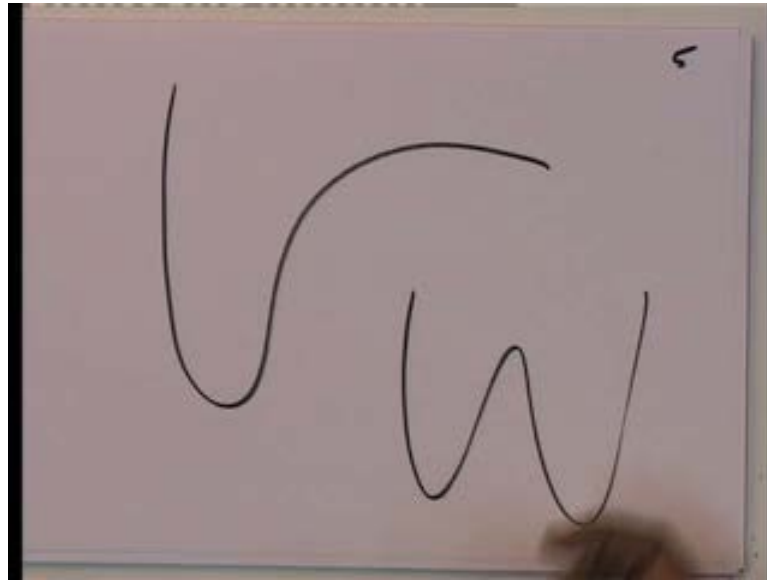
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Let us say, you have a function. Let us look at this plot. Let us say, you have some function, looks like this. So, this is the maxima, this is the minima. So, whenever there is a maxima and a minima, the function is changing, from increasing slope to decreasing slope; that is, changing its reduction rate, just curving. So, you, you can already find out the places where the function is going to curve; for you know, you know, in other words, it is like some other function, let us say, let us say, use the function, which might look like this.



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Some other function can look like, as we were discussing the free energy, some function can look like this. So, all these functions have minima or maxima, where we can, the function itself, is changing its slope, from either positive to negative or negative to positive. So, the slope is being changed. So, that is the main points, where it changes its direction. So, these points, we can, we can now figure out this points, by knowing whether there, where is maxima and where is minima, of any function. It will help us in figuring out the rough shape of the functions. So, I have, I am going to describe a recipe for plotting, sketching functions. The recipe is that, you have to do 1, 2, 3, 4, 5, 6 steps like the, like, there are few steps. If you do this steps, if you follow this steps...

It is like a protocol in Biology; if you follow this steps, very likely that, you will end up with some reasonable description of this plot of this sketch of this curve. So, from whatever the idea you learnt so far, you can follow this protocol, this recipe and end up with a sketch of any function, pretty much any function. So, let us see, what is the protocol, **right.**

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**BIOMATHEMATICS**

### Recipe for sketching $f(x)$

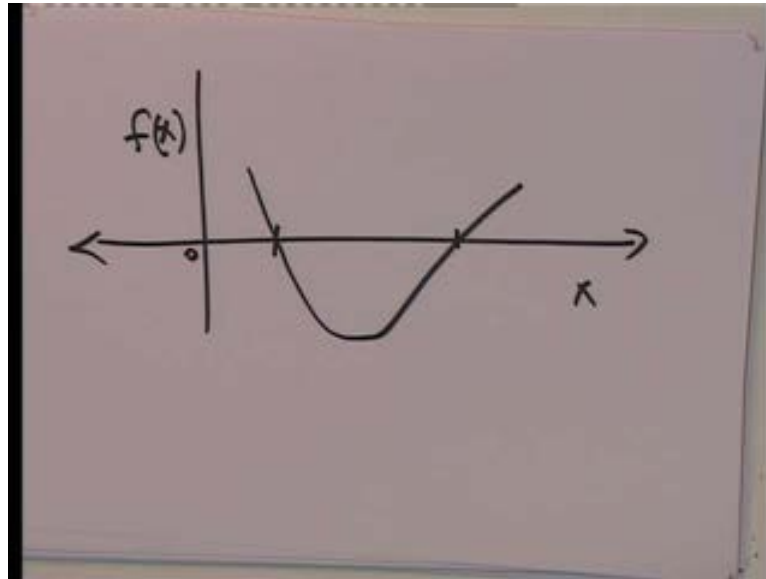
- Evaluate  $f(x)$  at 3 points:  $f(\infty), f(-\infty), f(0)$
- Find out the points where  $f(x)=0$
- Calculate the points where the function has maxima and minima (i.e.  $df/dx=0$ )
- Find out which one is a maximum ( $d^2f/dx^2 < 0$ ) and which one is a minimum ( $d^2f/dx^2 > 0$ )
- Evaluate the function at maxima and minima
- Make a schematic sketch using the above information

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So, let us see here. So, the recipe here is, let us have a look at this slide. The recipe here is that... So, recipe for sketching  $f$  of  $x$ , the first is point is that, evaluate  $f$  of  $x$  at 3 points;  $f$  equal to infinity,  $f$  equal to minus,  $x$  equal to infinity,  $x$  equal to minus infinity and  $x$  equal to 0. These are the three points, where, they are like, kind of extreme points, right. So, if you have any function  $f$  of  $x$ , the first thing we want to know is that, at infinities, like, when  $x$  equal to plus infinity or  $x$  equal to minus infinity or  $x$  equal to 0, how does this function, what is the value of this function? If we know that, we know that, faraway, the function either should go to 0, faraway, the function should go to infinity, faraway, as you go along the  $X$  axis, as in the  $x$  goes to infinity, the function should reach a particular value. So, we have a, we have an expectation, where should the function essentially and eventually end up, at this particular value.

So, the first thing, in this recipe, in this protocol is, take any function, calculate any function, like say  $x$  square or  $x$  cube; calculate what happens when  $x$  equal to infinity, when  $x$  equal to minus infinity and  $x$  equal to 0; this is the step 1. Step 2 is, as seen here is, find out the point where  $f$  of  $x$  equal to 0. So, find out the point where  $f$  of  $x$  equal to 0. So, that is, this points where...

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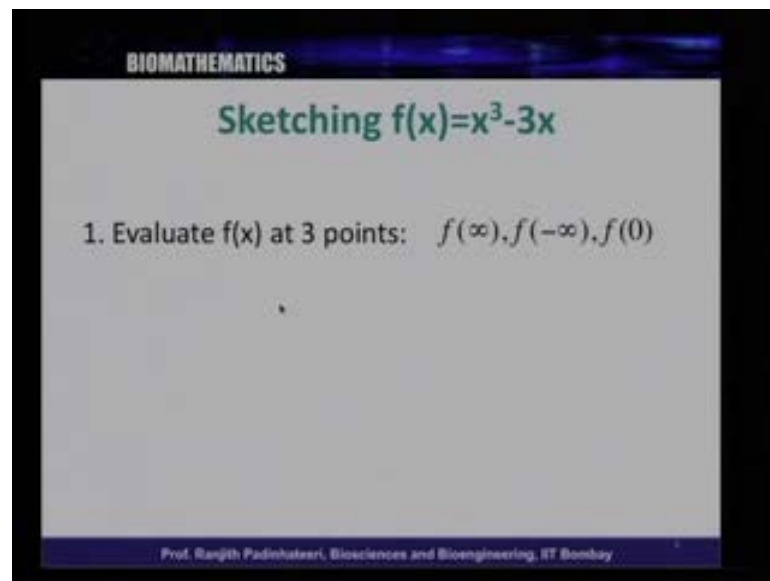
So, let us say, you have any function. So, this is  $x$  and this is  $f$  of  $x$  or  $y$  and first, we find out at, as we go to infinities, this ends, what is the value of  $f$  of  $x$  and then, second one, you find out, for what value of  $x$ , this  $f$  of  $x$  will be 0. So, that will give us some idea, whether the, where is the function crossing 0; if the function is, this is 0 and if it is crossing 0, at some particular point, if the value is 0, that means, it is touching 0 there; that means, it is likely that, it might cross 0 there. So, the second thing we do is, find out the value at which it will cross 0.

So, find out the points, where  $f$  of  $x$  equal to 0. The third thing is, calculate the points, where the function has maxima and minima. So, any function could have many maxima and many minima. So, as we learnt in the last few lectures, by calculating the derivative and equating it to 0, the point where the derivative is 0, is either a maximum or a minimum. So, this is the next thing we want to find out. The third thing you want to find out is, for what value of... The third thing you want to find out is, for what value of  $x$ , the function has derivative equal to 0.

So, find derivative, equate it to 0 and find out, what is the value at which this become 0; that is the third point. And, the fourth point is, you, **you** find many minima and which of this minima, which one is the maximum and which one is the minimum. If the second derivative is less than 0, we know that, it is a maximum and if the second derivative is greater than 0, we learnt that, it is a minimum. So, the next point is, find out, which one

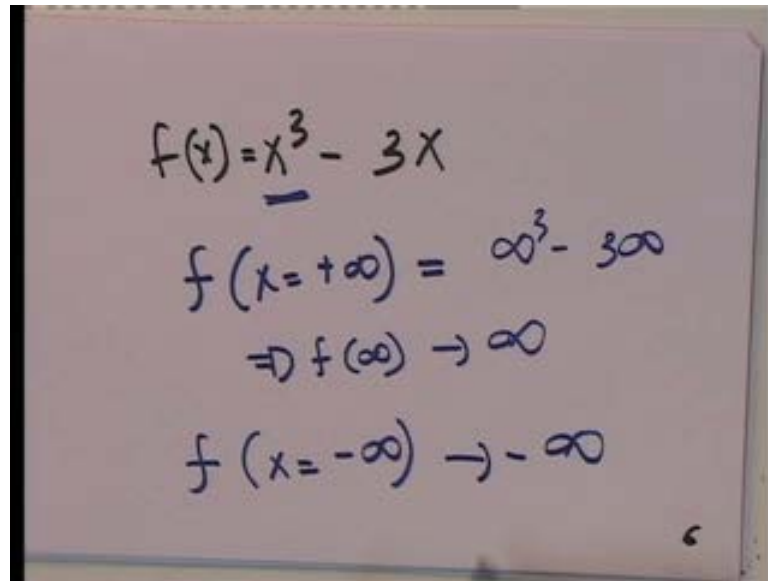
of it is a maximum and which one of it is a minimum. And, the next point is, evaluate the function at maxima and minima and make a schematic sketch using the above information. So, here is the recipe and what we will do now, in this lecture is, we will take one by one, take an example and we will follow this protocol, this, follow this recipe step by step and see what we get. So, there. So, thereby, we will learn it; you will learn it, how to do this.

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So, let us now take an example. So, the example that I want to study is,  $f$  of  $x$  equal to  $x$  cube minus  $3x$ . So, this is the example which I want to use today, basically, to teach you how to plot this function; and, the first instruction, the first in the protocol, the first instruction in the recipe is that, evaluate  $f$  of  $x$  at three points  $f$  equal to infinity,  $x$  equal to infinity,  $x$  equal to minus infinity,  $x$  equal to  $0$ . At this three points, you want to evaluate  $f$  of  $x$ .

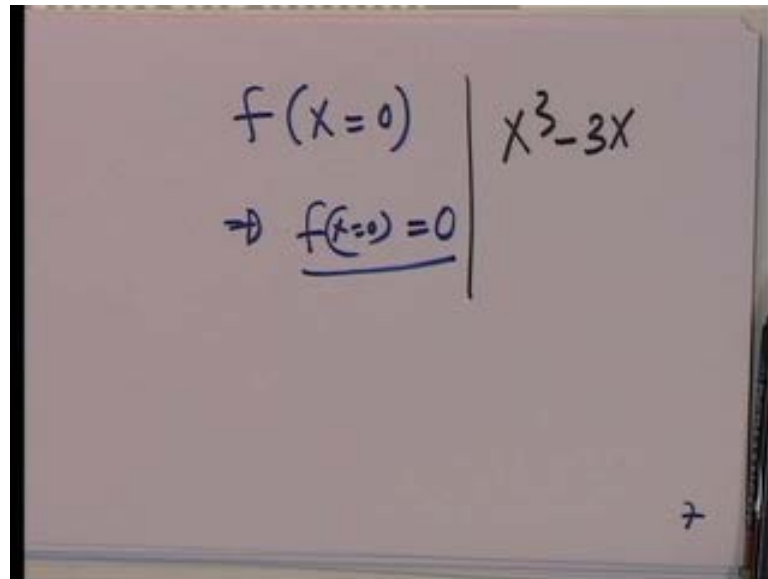
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$$f(x) = x^3 - 3x$$
$$f(x = +\infty) = \infty^3 - 3\infty$$
$$\Rightarrow f(\infty) \rightarrow \infty$$
$$f(x = -\infty) \rightarrow -\infty$$

So, let us start this. So, the function we have is  $x$  cube minus  $3x$ . This is our  $f$  of  $x$ . This is our function and what we want to find out is that, first, we want to find out,  $f$  at  $x$  equal to infinity. This is the first thing we want to find out. So, that means, you have to substitute for  $x$  equal to infinity. So, infinity cube minus 3 times infinity. So, you know that, anything in the infinity cubes will be like infinities; in the limit  $x$  going to infinity, where the  $x$  is very large, this is very likely that,  $f$  of infinity will go to infinity.

So, as the  $x$  tends to infinity, this function, likely to go to infinity. So, the next point we want to find out is at  $x$  equal to minus infinity, what will be the value? So, now, next one, we find,  $f$  at  $x$  equal to minus infinity. So, here, look at this function, if you put minus infinity here, minus infinity cube, infinity, infinity is, so three times multiplied. So, there will be a minus sign here. So, this term, which is dominating term, this is the dominating term, you all know that, we can guess that, when  $x$  is very large,  $x$  cube is a dominating term; like, for example, if  $x$  is 10,  $x$  cube is 1000 and  $x$  is just 10. So, 1000 is much larger than 10. So, whatever be the sign of this 1000, that will be the dominating sign. So,  $x$  cube is a dominating term and you can see, imagine that, as  $x$  goes to minus infinity, this function will go to minus infinity, because, this is how this cubic function goes. So, as  $x$  goes to infinity, this will go to minus infinity.

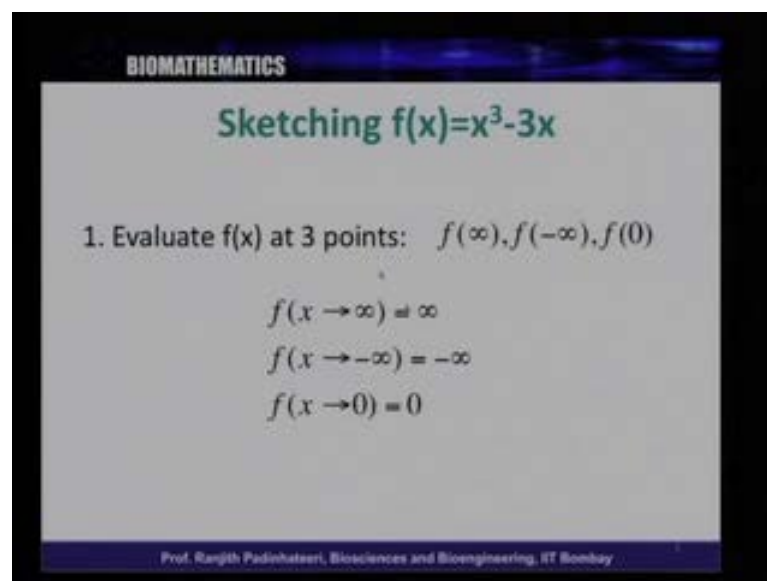
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Handwritten notes on a piece of paper. On the left, it says  $f(x=0)$  and below it  $\Rightarrow \underline{f(x=0) = 0}$ . On the right, separated by a vertical line, it says  $x^3 - 3x$ . In the bottom right corner, there is a small number 7.

Now, the next one is, what happens when  $f$  of  $x$  equal to 0. So, our function, as you know, let me write this function here, again. The function is,  $x$  cube minus  $3x$  is the function. At  $x$  equal to 0, you put 0 here, 0 here. So, this is 0 minus 3 into 0, 0. So,  $f$  of  $x$  equal to 0 implies, this is equal to 0, itself. So, the function is  $f$  of  $x$  equal to 0 is 0; the function is 0 there. So, what we saw now is that, at three points, at plus infinity, the function is infinity; at minus infinity, the function is minus infinity; at  $x$  equal to 0, the function is 0. So, this is the summary.

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**BIOMATHEMATICS**

### Sketching $f(x)=x^3-3x$

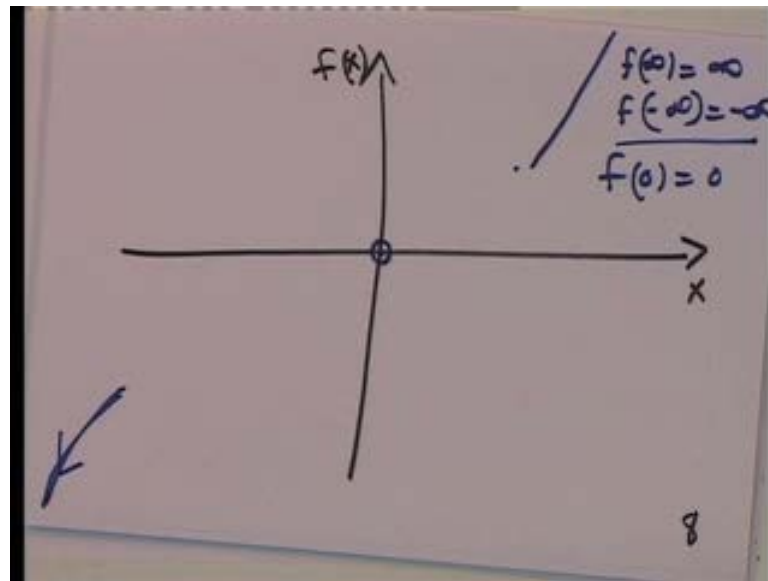
1. Evaluate  $f(x)$  at 3 points:  $f(\infty), f(-\infty), f(0)$

$$f(x \rightarrow \infty) = \infty$$
$$f(x \rightarrow -\infty) = -\infty$$
$$f(x \rightarrow 0) = 0$$

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So, look at this. The summary is that,  $x$  equal to infinity, the function is infinity.  $f$  at  $x$  going to minus infinity, the function is minus infinity and as  $x$  goes to 0, the function goes to 0. So, these are three limiting values; this is three points, where, for extreme values of  $x$  infinity and minus infinity, you have this function going to infinity and minus infinity and  $x$  equal to 0 is 0. So, we know this three values. So, what does this help, doing this, how does this help us?

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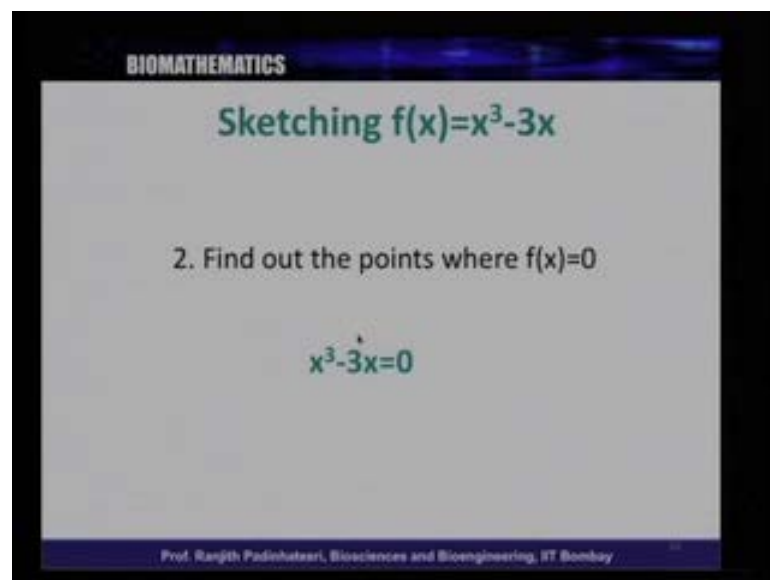
So, let us see, how does this helps us. So, let us plot. So, let us... This is X axis and this is  $f$  of  $x$ . Now, what we know? We know one thing that, when  $x$  is 0. So, this is  $x$  equal to 0. So, let us call it  $x$  equal to 0. So, we know that, at  $x$  equal to 0, the function is 0. So, it has, the function has to go through this particular value. So, we learnt that,  $f$  is equal to infinity is infinity,  $f$  is equal to minus infinity is minus infinity,  $f$  is 0 is 0. So, we know that,  $f$  of 0 is 0 and as this goes to a larger value of  $x$ , as  $f$  goes to infinity, as  $x$  goes larger and larger, the function should go to infinity.

So, as the  $x$  increases, the function should go to infinity. This is the way function, this is the only way the function, that one can go to infinity; like, somehow, as the  $x$  increases, function also should increase; then only, it can go to infinity. And, you know that, at 0, it has to be 0. So, from here, it has to go and increase somehow. And,  $f$  equal to minus infinity, as the  $x$  decreases, to goes to this way, the function has to go to minus infinity; this is what it says. So, this says that, as  $x$  goes to minus infinity, the function should also

go to minus infinity. So, the minus infinity is here, somewhere at the bottom. So, the function should, as the  $x$  goes, the function will go to minus infinity. So, the function will go to minus infinity. So, these two edges, these two ends, are clear.

At plus infinity, it has to go to infinity; at minus infinity, it has to go to minus infinity; at  $x$  equal to 0, it has to be 0. So, these three things are clear. Now, how is it, this in between here, which we do not know; which we will find out. So, but we got some clue already that, a three ends, the function will go to minus infinity, plus infinity, at 0, it is 0. So, it has to go through this point. So, this much is clear. Now, let us look at the next point in the recipe.

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So, the next point in the recipe is that, find out the points, where  $f$  of  $x$  is equal to 0. So, find out the points, where  $f$  of  $x$  equal to 0. So, the points where the function is 0; that means, the points where  $x$  cube minus 3  $x$  is 0. So, let us see, where are the, when is the  $x$  cube minus 3  $x$  is 0.



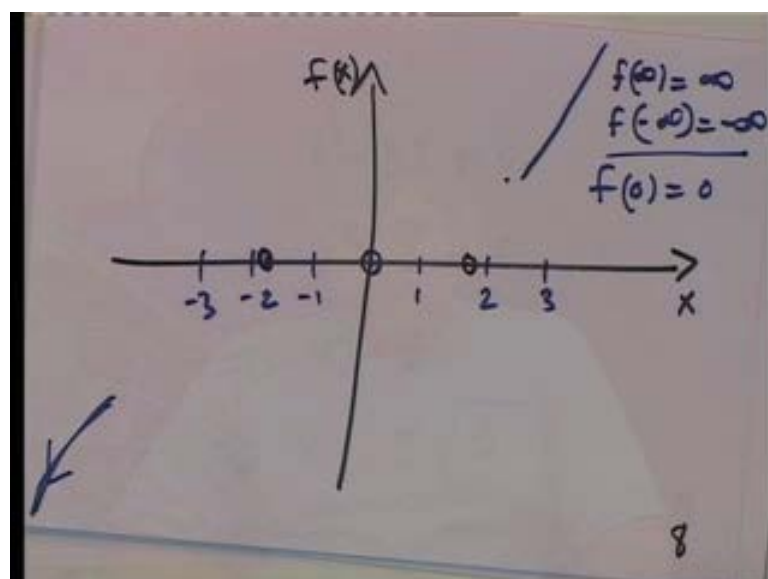
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$$\begin{aligned}x^3 - 3x &= 0 \\ \Rightarrow x^2 - 3 &= 0 \\ \Rightarrow x^2 &= 3 \\ \Rightarrow x &= \pm \sqrt{3}\end{aligned}$$

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So,  $x^3 - 3x = 0$  implies... So, there is an  $x$  and  $x$ , you can take out. So, you divide throughout by  $x$ . So, you have  $x^2 - 3 = 0$ . I can divide this term, this term and this term, by  $x$ . So, you will get that,  $x^2 - 3 = 0$ . This implies that,  $x^2 = 3$ ; because, I can take this 3 to this side. This implies that,  $x = \pm \sqrt{3}$ . So, when  $x$  is plus or minus square root of 3, the function is 0. So,  $x = \pm \sqrt{3}$  is what? Square root of 4 is 2. So, square root of 3 is just below 2. It is like, 1.7 something. So, when  $x$  is just below 2, just, you will have this function  $f$  of  $x$ , which is 0. So, let us look in this plot.

(Refer Slide Time: 29:27).



So, here, you have x equal to 0, here you have x equal to 1, here you have x equal to 2, here you have x equal to 3, so on and so forth and you have x equal to minus 1, x equal to minus 2, x equal to minus 3 and so on and so forth. So, what we found is that, when x is about square root of 3, which is about 1.7, which is very close to 2, somewhere here, the function should be 0. So, at this plus or minus square root of 3, at plus square root of 3 and minus square root of 3, the function should have hit 0; the function should pass through this point. This much we understood. So, and the next one we want to find out is that...So...So, let us look at, what is the next thing in the recipe.

(Refer Slide Time: 30:17)

BIOMATHEMATICS

Sketching  $f(x) = x^3 - 3x$

2. Find out the points where  $f(x) = 0$

$$x^3 - 3x = 0$$
$$\Rightarrow x = 0, x = +\sqrt{3}, x = -\sqrt{3}$$

Prof. Raghav Padinhateeri, Biosciences and Bioengineering, IIT Bombay

So, the next thing in the recipe is that find out...So, this is the, what we found that, x equal to three points. So, even at x equal to 0, there is, sorry, I forgot to say one thing that, even at x equal to 0, if you have put x equal to 0, you still get the function 0. So, even, three points. So, if you look at this, this point, this point and this point, these are the three points where the function will reach 0. So, these are the three points where the function is 0.

(Refer Slide Time: 30:57)

BIOMATHEMATICS

Sketching  $f(x)=x^3-3x$

3. Calculate the points where the function has maxima and minima (i.e.  $df/dx=0$ )

→  $df/dx=3x^2-3=0$

Prof. Rangh Padinhateeri, Biosciences and Bioengineering, IIT Bombay

And, the next one is, the next thing in the recipe is that, calculate the points where the function has maxima and minima. So, how do we find out, what does it mean, that is, if you calculate  $d f$  by  $d x$ , that is the derivative and equate that to 0, wherever this derivative is 0, those points are the points where you have either maxima or minima. This is one thing which we learnt before. You calculate the derivative, equate that to 0; the points where you, where the derivative is 0, you have maxima and minima. So, now, what is  $d f$  by  $d x$ ? Let us go back and learn once more, what is  $d f$  by  $d x$ .

(Refer Slide Time: 31:39).

$$f(x) = x^3 - 3x$$
$$\frac{df}{dx} = 3x^2 - 3$$
$$\Rightarrow 3x^2 - 3 = 0 \Rightarrow 3x^2 = 3$$
$$\Rightarrow x^2 = 1 \Rightarrow x = \pm 1$$

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So, as we learned,  $x$  is equal to  $x^3 - 3x$ , **sorry**,  $f$  of  $x$ , this is  $f$  of  $x$  equal to  $x^3 - 3x$ . Derivative, which is  $df$  by  $dx$  is equal to, what is the derivative of this function? So, derivative of  $x^3$  is  $3x^2$ ; this is what we learned,  $x^n$  has derivative  $n x^{n-1}$ , minus the derivative of  $3x$  is  $3$ . So, the derivative of this function is  $3x^2 - 3$  and we want to find out, where is  $3x^2 - 3$  equal to  $0$ ; the point, the value of  $x$  at which this derivative is  $0$ . What we want to find out? We want to find out the points of, the values of  $x$ , where  $3x^2 - 3$  is  $0$ . What does this mean? So, I can take this  $3$ , this side. So, I want... So, this would imply, this would give that, this means that,  $3x^2 = 3$ . So, if I can take this  $3$  this side, this, what does implies is that,  $3x^2 = 3$ . So, I can cut this  $3$  and  $3$ , which is means that,  $x^2 = 1$ . When  $x^2 = 1$ ,  $3x^2 = 3$ , which implies that,  $x$  is plus or minus square root of  $1$ , which is  $1$  itself.

So, when  $x$  is plus or minus  $1$ , you have  $x^2 = 1$  and  $3x^2 = 3$  and  $3x^2 - 3 = 0$ ; that means, when  $x$  equal to plus  $1$  or minus  $1$ , the derivative  $df$  by  $dx$  is  $0$ . So, we learnt that, at  $x$  equal to plus  $1$  or and minus  $1$ , you have an extremum; you have, you have extrema, you have either a maximum or a minimum. So, there are two extrema; we do not know, if it is maxima or minima yet; but we know that, we know that, this, at  $x$  equal to plus  $1$  or minus  $1$ , there is either a maxima or a minima. So, that much, we found out. So, let us go back to this curve. So, at this point,  $x$  equal to plus  $1$  and  $x$  equal to minus  $1$ , at this point and this point, you have either a maxima or a minima, but we want to find out, whether it is a maxima or a minima. So, that is the next thing in the recipe.

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BIOMATHEMATICS

### Sketching $f(x)=x^3-3x$

3. Calculate the points where the function has maxima and minima (i.e.  $df/dx=0$ )

→  $df/dx=3x^2-3=0$

⇒  $x = +1, x = -1$

Prof. Rangth Padinhateeri, Biosciences and Bioengineering, IIT Bombay

So, let us... So, what we did find so far,  $x$  equal to plus 1. So, we have to find out this. So, we found that  $x$  equal to plus 1 or minus 1, we have maxima or minima. Now, how do we find out, where is, whether it is a maxima or a minima?

(Refer Slide Time: 34:39)

BIOMATHEMATICS

### Sketching $f(x)=x^3-3x$

4. Find out which one is a maximum ( $d^2f/dx^2 < 0$ ) and which one is a minimum ( $d^2f/dx^2 > 0$ )

→  $d^2f/dx^2=6x$

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So, the way to find out is that, find out which one is the maxima, which, which one is the maximum and which one is the minimum. So, you have two extremas here, plus, at plus 1 and minus 1. Now, we want to find out, which of this is a maximum; whether it is a maximum; if it is a maximum or which one is the minimum. Now, the

way to find out is that, calculate the second derivative  $d^2f/dx^2$ , and if it is greater than 0, it is the minimum; if the second derivative is less than 0, it is a maximum. So, let us, this is what is written here. If  $d^2f/dx^2$  is less than 0, it is a maximum and it is a minimum, if  $d^2f/dx^2$  is greater than 0. So, what we want to find out is,  $d^2f/dx^2$ .

(Refer Slide Time: 35:35)

$$f = x^3 - 3x$$

$$\frac{df}{dx} = 3x^2 - 3$$

$$\frac{d^2f}{dx^2} = 6x$$

$$x = +1$$

$$\frac{d^2f}{dx^2} = 6x = 6(1)$$

$$= \underline{6} > 0$$

$$\Rightarrow \text{a minimum}$$

So, let us have a look at it. So, we have, function is  $x^3 - 3x$ , and we found that, this is our  $f$  and we found that,  $df/dx$  is  $3x^2 - 3$ , and  $d^2f/dx^2$ , another derivative of this. So, what is the derivative of  $3x^2$ ?  $x^2$  has a derivative  $2x$ ; so,  $2$  into  $3$  is  $6$ ; so, this is  $6x$  and derivative of  $3$  is  $0$ . So, the second derivative is  $6x$ . So, that is what we have written here, the  $d^2f/dx^2$ , the second derivative of this function is  $6x$ . And, we found that, when  $x$  equal to plus  $1$ , it is something, either a maxima or a minima and  $x$  equal to minus  $1$ , it is also a maxima or minima.

So, now, let us substitute  $x$  is equal to plus or minus  $1$  here. So, what we want, we, we know that, at  $x$  equal to plus  $1$  it is either a maxima or a minima. So, let us substitute  $x$  equal to plus  $1$ . So, you have  $d^2f/dx^2$  equal to  $6x$  is equal to  $6$  into  $1$ . So, we substitute  $x$  equal to  $1$ . So, you get  $6$ . So, which is greater than  $0$ . So, at  $x$  equal to  $1$ , the second derivative, that is,  $6x$  is greater than  $0$ . Because, at  $x$  equal to  $1$ ,  $6x$  is  $6$ . So,  $6$  is greater than  $0$ . So, at  $x$  equal to plus  $1$ , the second derivative is greater than  $0$ . This

implies that, a minima, it is a minimum. Whenever the second derivative is greater than 0, it has to be a minimum. Now, at, let us have a look at the next one which is...

(Refer Slide Time: 37:30)

The image shows a whiteboard with handwritten mathematical work. At the top, the second derivative is given as  $\frac{d^2f}{dx^2} = 6x$ . Below this, two cases are analyzed: at  $x = +1$ , the second derivative is  $\frac{d^2f}{dx^2} = 6 > 0$ , which is concluded to be a minimum; at  $x = -1$ , the second derivative is  $\frac{d^2f}{dx^2} = -6 < 0$ , which is concluded to be a maximum. The number 12 is written at the bottom right of the whiteboard.

$$\frac{d^2f}{dx^2} = 6x$$
$$\text{at } x = +1 \Rightarrow \frac{d^2f}{dx^2} = 6 > 0 \Rightarrow \text{minimum}$$
$$\text{at } x = -1 \Rightarrow \frac{d^2f}{dx^2} = -6 < 0 \Rightarrow \text{maximum}$$

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So, we found that, the second derivative  $d^2f/dx^2$  is  $6x$ . At  $x$  equal to plus 1,  $d^2f/dx^2$  equal to 6, which is greater than 0. At  $x$  equal to minus 1, what do we get?  $d^2f/dx^2$  is 6 into minus 1,  $x$  equal to minus 1; we are putting  $x$  equal to minus 1. So, this is minus 6, which is less than 0. So, if it is less than 0, this would imply that, this is a maxima; here is a maximum. So, here, this implies that, it is a maximum here. Here, as we learnt, when  $x$ , at  $x$  equal to plus 1, you have a minimum. So, you have a minimum here and a maximum here.

(Refer Slide Time: 38:40)

**BIOMATHEMATICS**

### Sketching $f(x)=x^3-3x$

4. Find out which one is a maximum ( $d^2f/dx^2 < 0$ ) and which one is a minimum ( $d^2f/dx^2 > 0$ )

$\rightarrow d^2f/dx^2=6x$

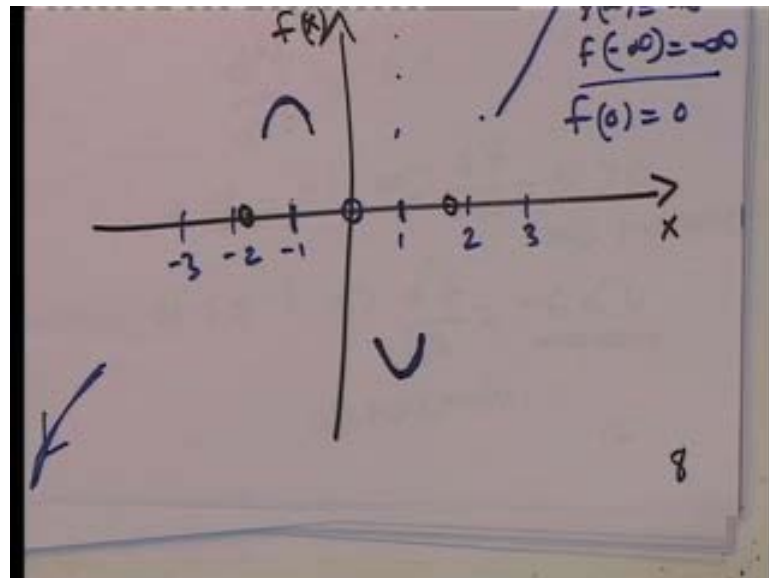
$\Rightarrow x = +1$  Is minima

$x = -1$  Is maxima

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So, let us look, this is what we, in the slide we show that, at  $x$  equal to plus 1, it is a minimum. So, it should be written as minimum and there is an arrow here, it should be written as  $x$  equal to plus 1, it is a minimum and  $x$  equal to minus 1, it is a maxima So, let us look at this plot once more. What did we learn? We learnt, let us look at this.

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So, we learnt that,  $x$  equal to plus 1, it is a minimum. So, here, at equal to plus 1, the function should have a minimum; that means, the function should have something like this. So, we do not know what, whether it is here or here or here, where is this minimum,



but we only know it is minimum, at some particular, at any of these points, we should have a minimum and at this particular point, you should have a maximum somewhere. You should have a maximum somewhere. We do not know, where it is; it is here or here or here; we do not know, where is this maximum, but we know that, at  $x$  equal to minus 1, you should have a maximum; the function should look like this; a (( )) curvature like this and at equal to plus 1, you should have a minimum, where the function should look like this. Now, what is the value at which this maximum, minimum should happen. So, we should evaluate the function at  $x$  equal to plus 1 and minus 1.

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BIOMATHEMATICS

Sketching  $f(x)=x^3-3x$

5. Evaluate the function at maxima and minima

At  $x=+1$ ,  
 $x^3-3x=-2$

At  $x=-1$   
 $x^3-3x=2$

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So, let us, the, next recipe. Let us go to the next recipe. So, here, next one says, evaluate the function at maximum, maximum and minimum. So, there are again error here. It should be, should read as, evaluate the function at maximum and minimum. So, at  $x$  equal to plus 1,  $x$  cube minus 3  $x$  is minus 2. And so, at  $x$  equal to minus 1,  $x$  cube minus 3  $x$  is plus 2; this you can see. So, how do we see that? So, let us learn how do we see that.

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$$x^3 - 3x$$

$$x = +1 \Rightarrow 1^3 - (3 \cdot 1) = 1 - 3$$

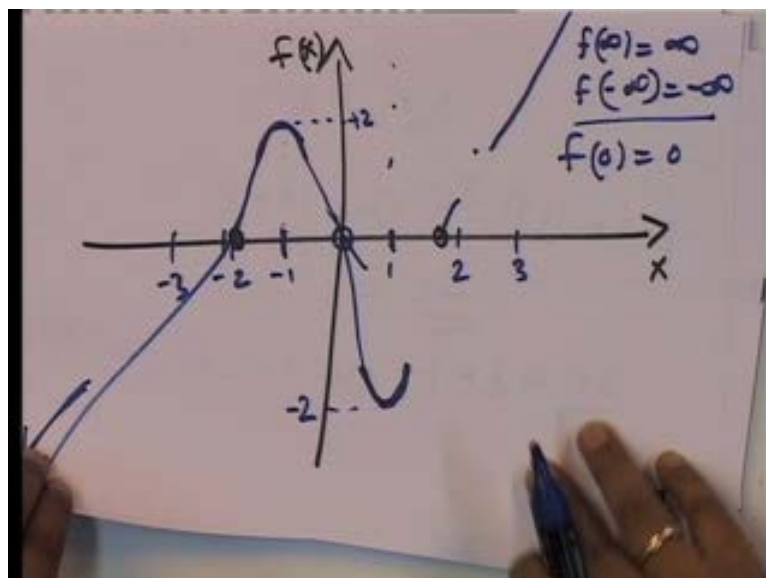
$$= \underline{\underline{-2}}$$

$$x = -1 \Rightarrow -1 + 3 = \underline{\underline{+2}}$$

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So, the function is  $x$  cube minus  $3x$ . So,  $x$  equal to plus 1 implies that, 1 cube minus 3 into 1, which means 1 minus 3, which is minus 2. So, at  $x$  equal to plus 1, the function is minus 2; and  $x$  equal to minus 1, the function is, minus 1 cube is minus 1; minus 3 into minus 1 is, minus 3 into minus 1 is plus 3. So, this is plus 2. So, at  $x$  equal to plus 1, it is minus 2 and  $x$  equal to minus 1, it is plus 2. So, what does this mean? This means that, at  $x$  equal to plus 1, the function is at minus 2; the minimum is at minus 2.

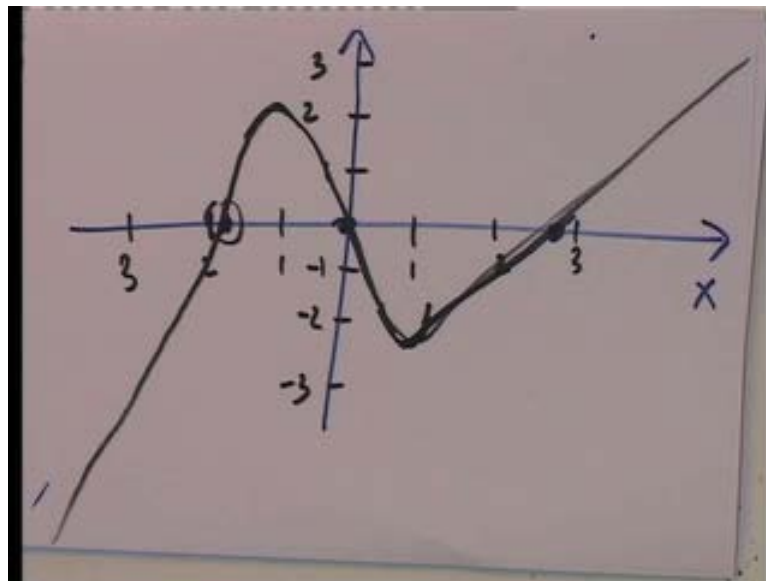
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So, this has to be minus 2. So, this has to be minus and  $x$  equal to minus 1, this maxima happens at plus 2. So, at plus 2, there is a maxima and at minus 2, there is a minima. So, we know this much thing. You know a lot of things now. We know that...So, have a

look at this. We know that, at the ends, it goes like this and we know that, there is a maxima here and there is a minima here. And we know that, it should go through 0 here; it should go through a 0 here. So, if you join all these together smoothly... You should, you should, you should... So, let us, let us join all these together. So, let us, let us draw all these knowledge. Let us combine all this knowledge into a nice graph. So, let us combine all these knowledge.

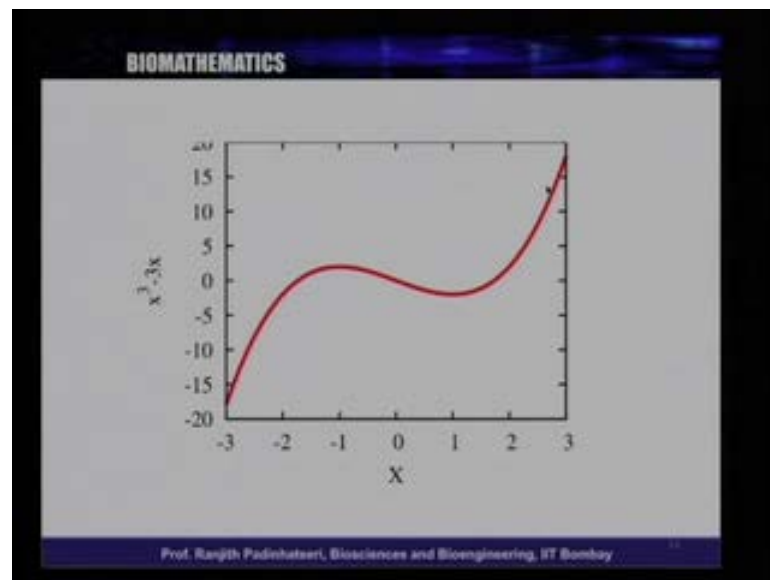
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So, what do we know? So, let us again draw this axis. So, this is X and this is f of x. So, now, we know that, at x equal to... So, what do we know? We know few things. We know that, the points, where it is 0 is that, at root 3, square root of 3, that is here, somewhere here and somewhere here. So, this is like... Let, let us call it, this is 1. So, let us call this is 1; this is 2; this is 3 and this is 1, 2, 3 and this is plus 1; this is 2 and 3 and this is minus 1, this is minus 1, minus 2, minus 3 and so on. We know that, at square root of 3, plus or minus square root of 3, the function is 0. So, somewhere here and somewhere here, the function is 0; here also the function is 0. So, these are the three points where the function is 0 and at the, at the, as it goes far away it should go to infinities, it should go to infinities. And, we also know that, at x equal to plus 1, there is a minima at minus 2. So, x equal to plus 1, there is a minima at minus 2. So, we know that, there is something like this here.

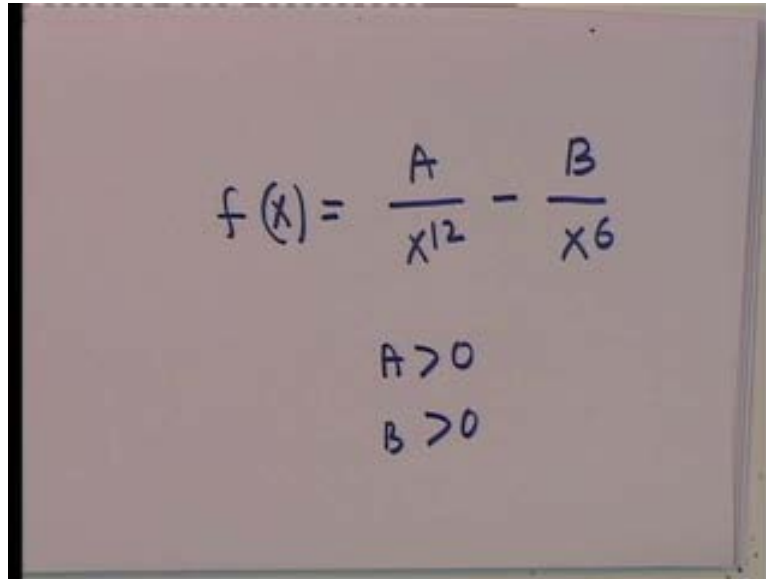
Something like this here and we know that, there is a maxima here and it should pass through this 0, and it has to have a maxima and a minima and then, again it should pass through this, this is another point, where it should pass through 0. So, it should pass through this and it should go to infinity. And, again here, minima and then, it should pass through this and should go to infinity. So, this is some function, which has some maxima and minima and then, it should go to infinities at both the ends. So, the function should look like this. One maxima, one minima, one maximum, one minimum and at either ends, it should go to infinity and these are the points, where it should hit 0. So, knowing this much, we could just join together and this, the function will look like this.

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So, this is how the function looks like. So, there is a maximum, there is a minimum and it should look like this. So, this is how you schematically plot a function. So, this is one example, where you schematically plot a function. Now, we will take one more example and then, just discuss, how do we schematically plot this function. Now, that we learnt this one example, which is a  $x$  cube minus  $3x$  and the protocol, we have the protocol for plotting it, we should take another example. So, the example I am going to say is, the function which is very well known in various fields. And, this function basically, describes the interaction between two atoms. So, this is called Lennard-Jones potential. So, the function looks like this.

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A photograph of a whiteboard with handwritten mathematical expressions. The top line shows the function  $f(x) = \frac{A}{x^{12}} - \frac{B}{x^6}$ . Below this, two conditions are written:  $A > 0$  and  $B > 0$ .

So, the function which I am going to describe is  $f(x)$  is  $A$  by  $x$  power 12 minus  $B$  by  $x$  power 6. This is the function which we want to plot, for some particular value of  $A$  and  $B$  and we know that,  $A$  is some value greater than 0,  $B$  is some value greater than 0. This much we know. Some numbers,  $A$  and  $B$  are some numbers. It could be 6, 3, we do not know; any number, which is greater than 0. So, this is of, this is called a Lennard-Jones potential and this describes the interaction between two atoms. So, we will quickly go through this protocol and try and plot this function quickly. But you should take it as an assignment yourself, and try and plot it yourself, you, following the protocol that we described. But, let us just, quickly go through, go back to the protocol and then, see, how do we plot it.

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**BIOMATHEMATICS**

### Recipe for sketching $f(x)$

- Evaluate  $f(x)$  at 3 points:  $f(\infty), f(-\infty), f(0)$
- Find out the points where  $f(x)=0$
- Calculate the points where the function has maxima and minima (i.e.  $df/dx=0$ )
- Find out which one is a maximum ( $d^2f/dx^2 < 0$ ) and which one is a minimum ( $d^2f/dx^2 > 0$ )
- Evaluate the function at maxima and minima
- Make a schematic sketch using the above information

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So, the protocol we say here, is this. The first one is evaluate the function at three points, at infinity, at two infinities, plus infinity, minus infinity and 0.

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$\frac{A}{x^{12}} - \frac{B}{x^6}$

$x \geq 0$   
 $x \leq 0$

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So, let us start doing it. So, our function here, now, is that A by x power 12 minus B by x power 6. This is our function and if you put x equal to infinity, what happens. So, that is, now, one thing which we should, I should tell you, like, we should imagine one thing. So, we are plotting... This function basically, represents the distance between two atoms, that is, the interaction of two atoms. So, when you say two atoms, the closest the two

atoms can come together is 0; there is nothing called a negative distance between the two atoms. So, the two atoms can be faraway, where the distance is very large and, positive and very large that, that is, the distance is 10 millimeter or 10 micrometer or 10 nanometer. And then, they can come closer and closer, **closer** and closer, nanometer, micrometer, nanometer range and angstrom range and they can come maximum 0 distance; there is nothing called negative distance. So, we would not discuss the negative part. We will only discuss, we are only interested in the positive part. So, the X starts from 0 and goes to positive and we want to see how does this function look like, in this part. So, x is 0 or x is greater than 0, greater than or equal to 0

So, we are interested only in x is greater than or equal to 0. So, now, in that sense, in this recipe, f of minus infinity has no meaning; because, x does not go to infinity; it is not a, it is, it is not a physical thing for us. So, we will evaluate the function at f equal to infinity and f equal to 0. So, have a look at this function; have a look at the... At x equal to infinity, 1 over infinity is 0. Here is also infinity that the denominator. So, 1 over infinity, 0. At x equal to infinity, this function will go to 0. So, as the x goes to very large, the function should reach 0. So, this is 0 and this is positive. And, this is also positive. So, this is the origin 0, 0 point. So, as x goes very large, our aim is, that the function should reach 0; that is the first recipe. Second recipe is, find out the point, where f of x equal to 0. So, the next point is to find out, where this function is 0.

(Refer Slide Time: 50:05)

The image shows a whiteboard with handwritten mathematical steps. At the top, the equation is written as  $\frac{A}{x^{12}} - \frac{B}{x^6} = 0$ . Below this, an arrow points to the equation  $\frac{A}{x^{12}} = \frac{B}{x^6}$ , which is then rearranged to  $\frac{A}{B} = \frac{x^{12}}{x^6}$ . A second arrow points to a crossed-out version of the equation  $\frac{x^5}{x^{12}} = \frac{B}{A}$ , which is then simplified to  $\frac{A}{B} = x^6$ . The final result  $\frac{A}{B} = x^6$  is written with a hand holding a marker.

So, let us quickly do this, the recipe, the protocol number 2, which is, find out where A by x power 12 minus B by x power 6 equal to 0. This implies, what does this imply? This means that, A by x power 12 equal to B by x power 6. This implies that, x power 12, x power 6 by x power 12 is equal to, I can take this way, B by A. So, let, **let** us do it slowly; let us do it slowly. So, what does this imply? This imply, I can take x power 12 this side and x power 6 this side. So, **sorry**, x power 12, this side and B, this side. So, I can say A by B is equal to x power 12 by x power 6. So, this implies that, A by B is x power 6.

(Refer Slide Time: 51:14)

The image shows a whiteboard with the following handwritten text:

$$\text{When } x = \left(\frac{A}{B}\right)^{1/6}$$

$$f(x) = 0$$

$$f(x=0) = \frac{A}{0} - \frac{B}{0} = \infty$$

So, that, this essentially leads to the value, which is, when x is equal to A by B whole power 1 by 6, when x is equal to A by B whole power 1 by 6, f of x is 0. So, this is the value, where f of x equal to 0. Now, the next recipe thing says that, find out the, where it has a maximum or a minimum. So, just before that, we forgot one thing. We wanted to find out the function at x equal to 0. So, f at x equal to 0 is A by 0 minus B by 0, which is basically, infinity. So, at x equal to 0, the function is infinity. So, that we know. Now, we want to find out the derivative. So, what is the derivative of this function?



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The image shows a whiteboard with handwritten mathematical work. The first line is the derivative of a function:  $\frac{df}{dx} = \frac{d}{dx} \left[ \frac{A}{x^{12}} - \frac{B}{x^6} \right]$ . The second line shows the result of the differentiation:  $= -12A x^{-13} + 6B x^{-7}$ . The third line shows the derivative set to zero:  $\frac{df}{dx} = 0 \Rightarrow$ . To the right of this, there is a fraction  $\frac{x^{-13}}{x^{-7}} = \frac{12A}{6B}$ . The terms  $x^{-13}$  and  $x^{-7}$  are crossed out with a diagonal line, and the terms  $12A$  and  $6B$  are also crossed out with a diagonal line, leaving the simplified equation  $1 = 2 \frac{A}{B}$ .

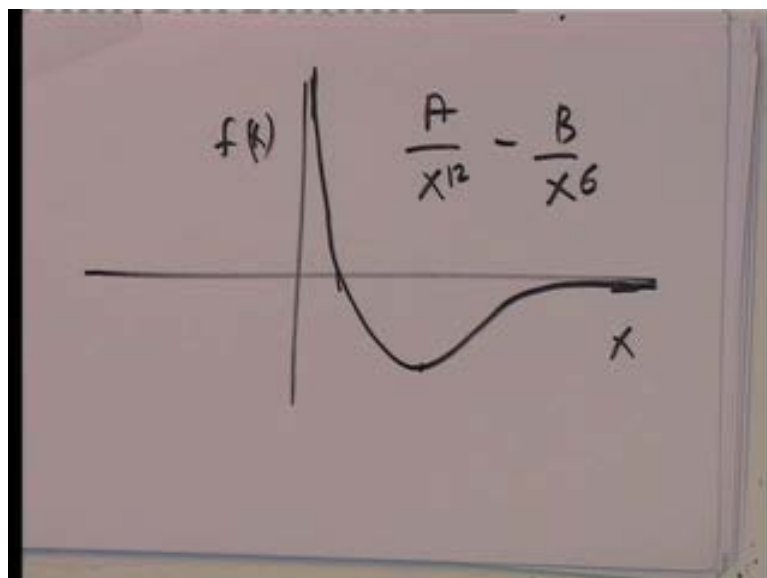
So, we want to find out the derivative of this function, which is d f of by d x, d by d x of A by x power 12 minus B by x power 6. So, I will quickly do this. So, x by, you can...So, basically, the derivative of this is A into minus 12 x power minus 13, minus B by, this is plus 6 x power minus 7. So, this is the derivative and d f by d x equal to 0 implies, we want to find out the derivative and equate it to 0. So, this, equal to 0. So, this equal to 0 implies, again, what does this imply? This implies that, x power minus is... So, we can take all this, this side. So, x power minus 13 divided by x power minus 7 is equal to 12 A by...So, you should, you should do this carefully. So, one should...What you want...Let us, let us do it carefully, little more. So, what we want is d f by d x equal to 0. So, let us equate this is to 0. So, what we want is, let us have a look at it.

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$$\frac{-\frac{2}{x^{13}}}{\frac{2A}{B}} = \frac{-\frac{6}{x^7}}{\frac{2A}{B}}$$
$$\frac{2A}{B} = x^6$$
$$x = \sqrt[6]{\frac{2A}{B}} = \left(\frac{2A}{B}\right)^{1/6}$$

So, we want minus 12 A by x power 13 equal to minus 6 B by x power 7. This is what it means. So, this means that, I can, this is, divide this and there are two and this says that, 2 A by B is equal to x power 6. So, x is equal to 2 A by B, square root of 6, 1 by 6 or, this means 2 A by B whole power 1 by 6. So, at this particular value, when x is 2 A by B whole power 1 by 6, the derivative is 0. Now, you will, you substitute this...Now, you want to find out the second derivative. So, what you should do is that, find the second derivative and substitute it and you will see that, it is a minima, it is a minimum at this particular value. So, at this value of 2 A by B whole power 1 by 6, it is a minimum.

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So, we learned a few things. We learnt that, at  $x$  equal to 0 is infinity. So, the function should go to infinity; at  $x$  equal to infinity, it should go to 0 and there is a minimum somewhere here and we also will learn that it crossed 0 here; there is a point, where it crosses 0. So, if you use all these information and combine this, what you will find, that it crosses 0, there is a minimum here and it should go to 0, like this. So, you will get something like this, as  $f$  of  $x$  versus  $X$ . So, this will be  $A$  by  $x$  power 12 minus  $B$  by  $x$  power 6. So, I am doing it in a hurry, because we have, today, in this lecture, I already described you a protocol and an example and I quickly wanted to tell you that, if you use this example, use this as an assignment or use it as a take home, take home question and do this plotting yourself and you will find a plot, which look like this. I already explained to you, this is 0, this is infinity; there is a minimum here, minimum here and it crosses 0 at one point.

So, all this is clear to you. So, this is the thing, which, the answer will look like this. So, do it yourself. **So, what, the...** To summarize, what we learnt is, we will, first, we briefly discussed some applications by pulling DNA, unzipping of DNA and the force is basically, the derivative of, derivative of free energy and distance, force and distance are derivatives of free energy and  $dG$  by  $df$  is distance. Then, we discussed a protocol, a recipe to plot, to sketch functions by, by using, calculating, where is the maximum, where is the minimum, where are the minima and maxima and where will be 0s of the function, at plus or minus infinities, whether it will go to infinity or what will be the value of the function. And, knowing the few things and combining this knowledge, we can roughly sketch the behavior of the function. So, we learnt this much. You should do many such examples yourself; have a look at the text book referred in the syllabus and you should learn this, to plot many more functions.

So, in this lecture, we will stop here. In the next lecture, we will continue with more different things in calculus. So, at this moment, we stop here. **Thank you.**