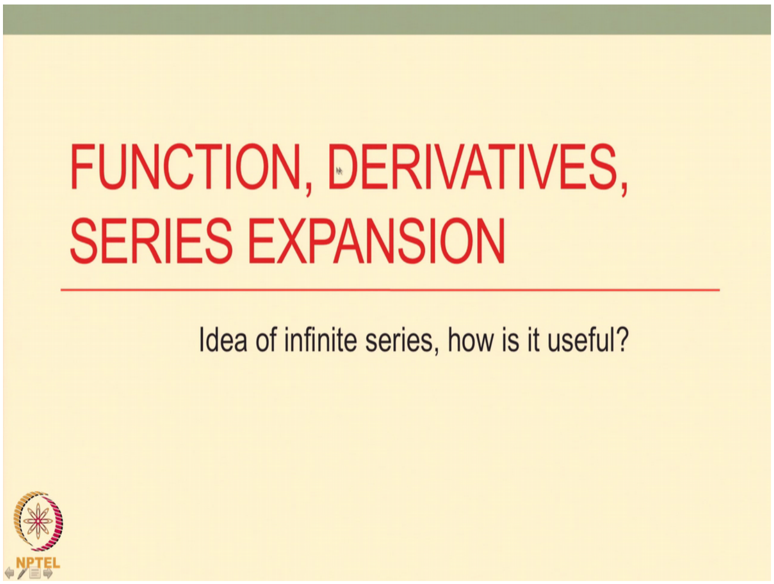
Introductory Mathematical Methods for Biologists
Prof. Ranjith Padinhateeri
Department of Biosciences & Bioengineering
Indian Institute of Technology, Bombay

Lecture - 14
Function, Derivatives and Series Expansion

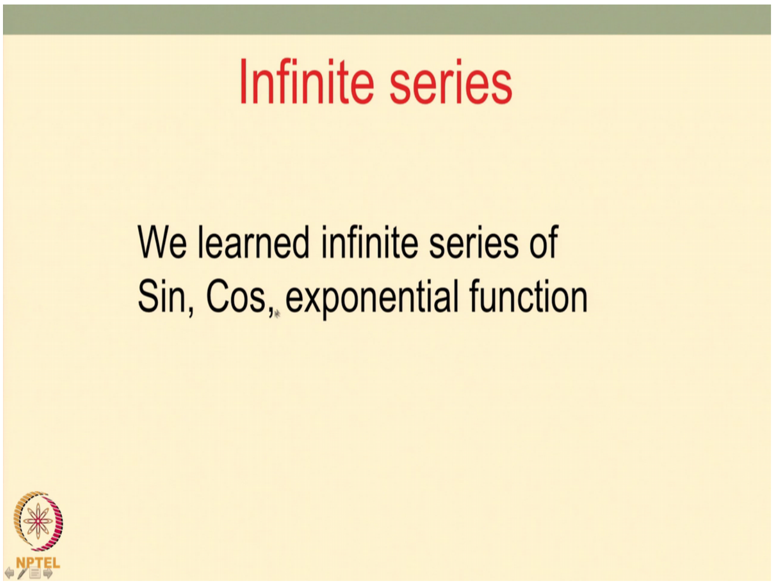
Hi, welcome to this lecture on mathematical methods for biologists today's topic is function, derivatives and series expansion.

(Refer Slide Time: 00:24)



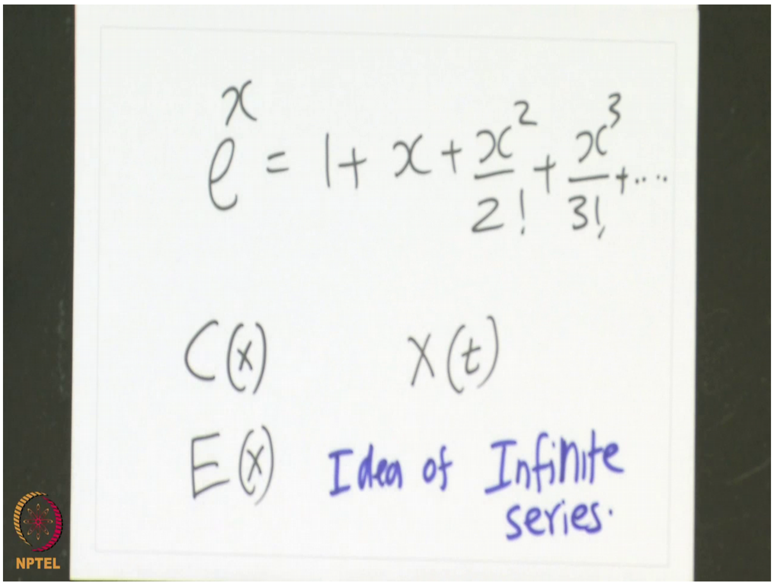
So, in this lecture we will discuss the idea of infinite series once more, and what is the idea behind the infinite series and how is it useful, what is the use of this series. So, what we learned is that, we learned infinite series for various functions.

(Refer Slide Time: 00:48)



We learned infinite series of sin, cos and exponential function, and we have learned for example, that e power x can be written as 1 plus this is something that we learned e power x can be written as 1 plus x plus x square divided by 2 factorial plus x cube divided by 3 factorial plus dot dot up to infinity. So, finally, we will have x power 10 x power 100 x power this whole thing is e power x.

(Refer Slide Time: 01:02)

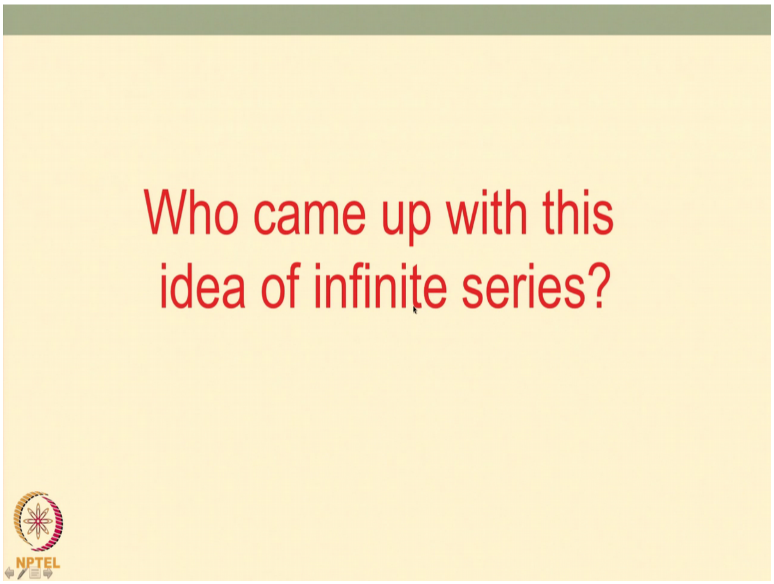


Now, this kind of infinite series, where did it come from? The first person is who started with this idea that any function can be kind of written as an infinite. So, it turns out that any function can be written as an infinite series like this any function and this is very useful in general for science also in biology because, many things that what we want to know in sciences and in biology, if you want to know for example, concentration as a function of x . So, for example, you want to know C of x. So, you want no concentration at some point x, if you know some other information or we want to know energy as the function of x at some particular x, you know energy or you want to know the position as the function of time.

So, this is concentration energy position. So, we want to know all of these functions. If we know some ideas in mathematics can we guess this function, do is it useful to understand these functions these are the questions that would come to anybody's mind can I know this function, can I know the energy function just like that by knowing some ideas from calculus.

Can I guess the energy function, can I write down the energy function, can you know the position if I know some information right. So, this is the thing that anybody would want to know. So, for this this infinite series is very useful. So, we would use this idea from infinite series. So, idea of infinite series. So, first of all who. So, the obvious question is who started this idea who where did it come from that. Any function more many functions can be expanded as infinite series right.

(Refer Slide Time: 03:18)



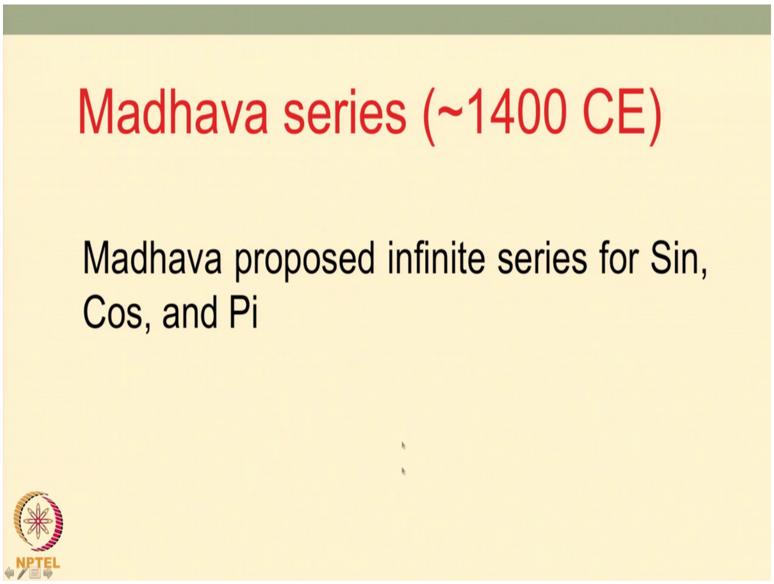
So, this is a question that who came up with this idea of infinite series. It turns out that this idea was first discovered in India in around 1400. So, this idea was first proposed by mathematicians in Kerala.

(Refer Slide Time: 03:33)

A part of south India a part of India around 1400 CE of course, we may not know the exact date so, but the manuscripts that know got from Kerala which has as old as 1400 1500 CE describes the infinite series of sin cos and all that. So, there is something called there were in around this time, the medieval times 1400 to 1500 CE

There was a school there was a group of scientists who formed who knows known as Kerala school of astronomy and mathematics, this was a group of mathematicians and astronomers who lived in this era from 1400 CE to 1500 CE, and one of the prominent person in that his name is Madhava. Ma and the place is called Sangamagrama. So, madhava of sangamagramma in Kerala first proposed this kind of infinite series first around 1400 CE.

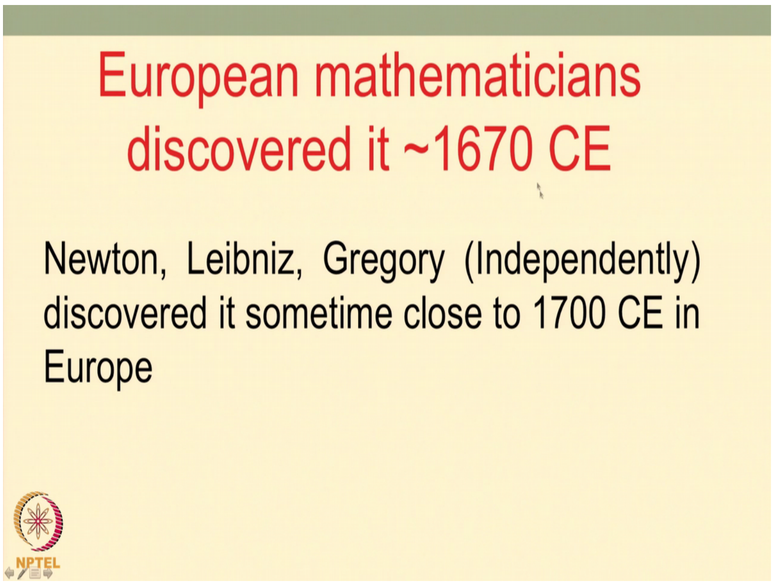
(Refer Slide Time: 04:39)



So, madhava proposed series for sin cos n Pi. So, pi can be written as tan inverse x. So, you should think about how Pi can be written as sin inverse x. So, he first proposed the madhava proposed this series for sin cos and tan inverse x, which is related to the Pi.

So, using this idea we do not know how whether anybody else knew this idea at the time, but certainly the manuscript that we know now we have got now, clearly shows that this was known to them and there was detailed description of all this. So, later about 200 years later, close to 1700 CE, CE means common era which same as AD right.

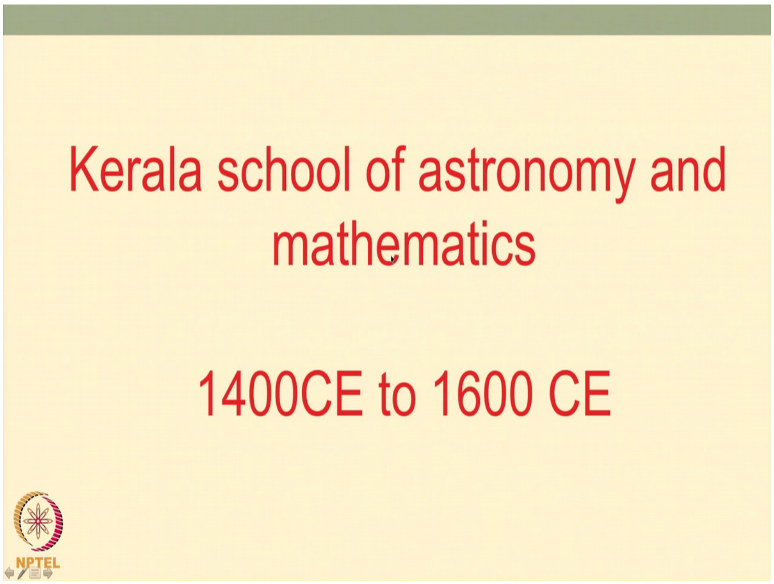
(Refer Slide Time: 05:34)



So european mathematicians discovered it around 1670 in the common era which is CE which is AD. Newton Lebanese Gregory they all worked independently, and discovered these series like they all discovered different series.

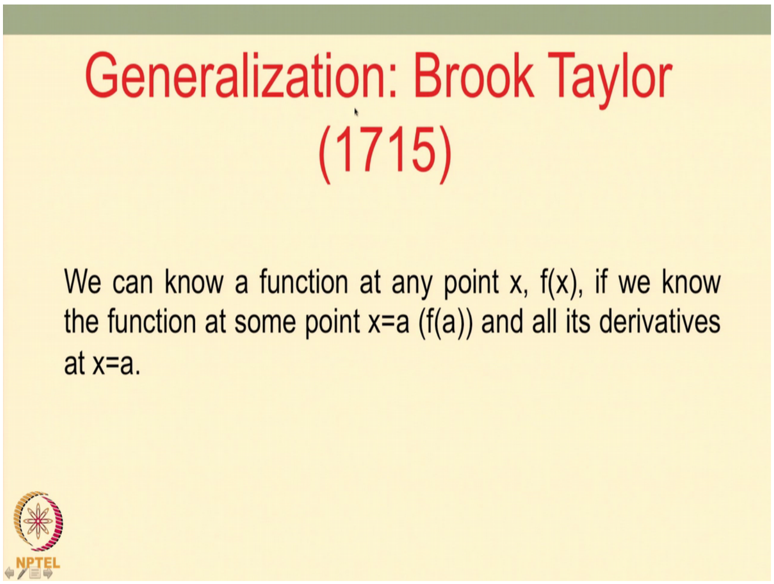
So, this Lebanese series Gregory series, but they are all infinite series some sometime around seventeen 100 CE, CE is Common Era in Europe this was discord. So, probably this was discovered first around 1400 -1500 CE about 200 years before Europe in India, but whether this was spread to Europe or not we do not know precisely, but a British civil servant who worked in Kerala that time, he was collecting manuscripts old manuscripts of various parts of India and when he read this he found out this school in Kerala Charles wish, and from that people understood about this and now I urge all of you to go to Google and search for Kerala school of astronomy and mathematics.

(Refer Slide Time: 06:38)



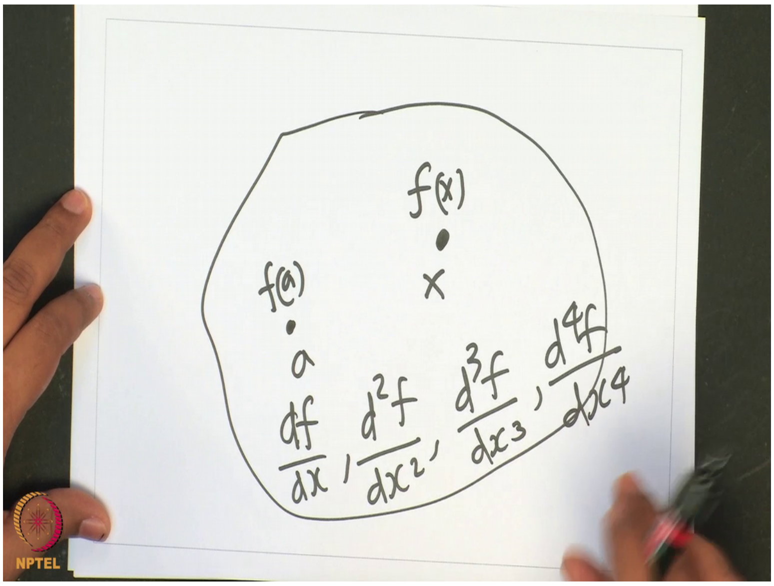
In the medieval Kerala it is also called Kerala school of mathematics, which was flourished around this 200 years period from around one 1400 CE to 16 100 CE, there are a bunch of very famous mathematicians, who did excellent work pioneering work couple of see there is before what it was discovered in Europe and elsewhere.

(Refer Slide Time: 07:16)



So, but what we now use as an infinite series which is very commonly used is called the Taylor series and this was generalized addition of this series by person called brook Taylor a British scientist, I think surround 1715 CE and we what Taylor found is that, we can know a function at any point x, that is we can find f of x at any point x, if we know the function at some point a and all its derivative at x equal to a. So, this is something very useful we want to do any function. So, this is something which is very useful and let me describe this little bit carefully. So, we want to know.

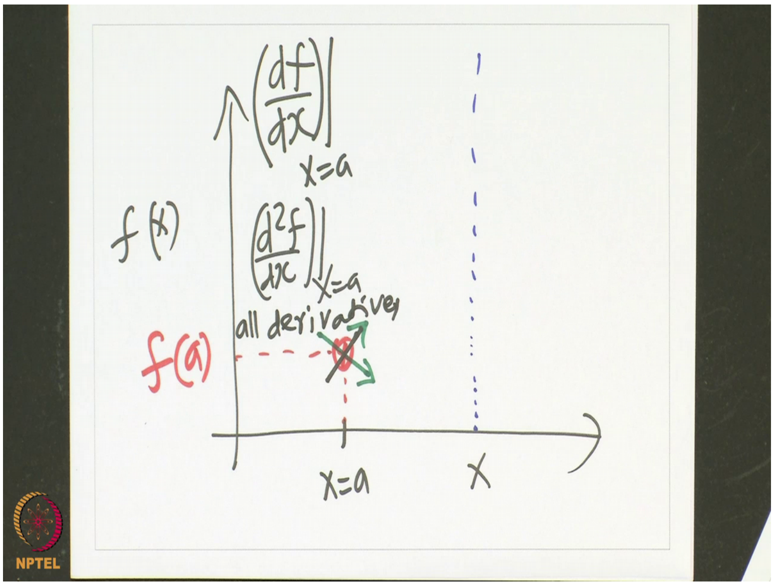
(Refer Slide Time: 08:00)



So, think about somewhere any. So, you want to know the function value at this point x, you order the value of this function this one if I know this function some other point which is called a, if I know the value of the function here can I know the value of the function here . So, can I find out the value at x, if I know the value at a.

It turns out that we can find, and how to find this is what is the Taylor series. So, the Taylor series says the following to know the function at x, you have to know the function at a and all its derivatives at a. So, if you have to know df by dx at a, you have to know d square f by dx square at a, d cubed f by dx cubed at a, d power 4 f by dx bar 4 at a. If I know all this derivative at a, at this point and the function we can calculate the value of the function at this point. So, let us understand this in a different way if I plot this. So, we would typically plot x verses f of x. So, at some point x. So, let us say this point x.

(Refer Slide Time: 09:13)



The function could have any value. So, the value of the function the y value, the value of the function could be anything it could be here or it could be here or it could be here we want to know where this function is the value is here or here or here or here what is the y value we want to know that. So, that is what we want to know f of x, but we can know that if I know the value at some other point here, which is x equal to a. So, if I know that at x is equal to a the value is this, the next the value here could be the function would be here could be here or here it could be anywhere on this line.

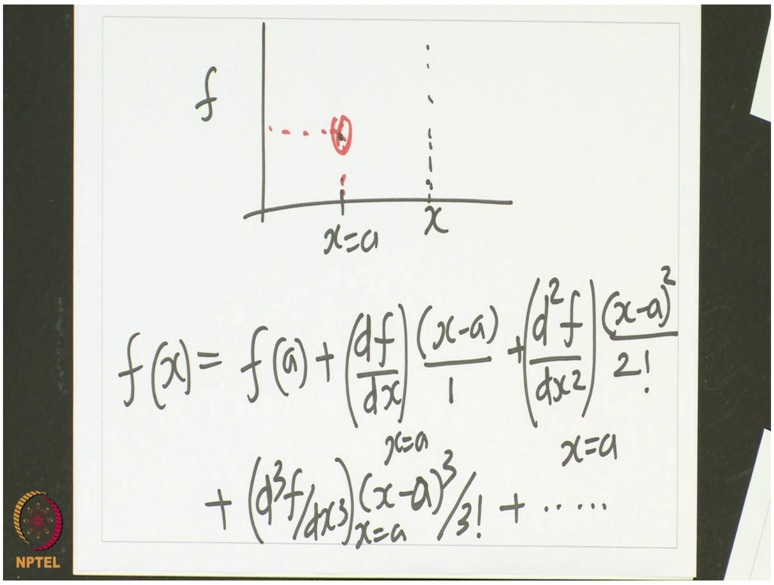
The next point here could be here or here or here or here we do not know anything. We only know this value of this function at this point f of a. So, we know this f at a; it is not enough to know this function at a of course, if I just know this point I cannot guess, where this is I have to know the derivative that is the slope.

If I know the slope, if I know df by dx, think about it if I know the df by dx what do I know? So, if I know the df by dx at x equal to a, if I know that the df by dx at x is equal to a is positive, then it is going to be the slope local slope is going to be like this the local slope is going to be like this; that means, the function is likely to go up. If the local slope was if the function is negative the local slope is going to be like this if the function is if the df by dx is negative then the local slope is going to be like this.

So, then the function is going to decrease. So, that is the local slope first of all we will give you the direction whether it is going to go up or going to go down and therefore, this is very useful quantity. I hope you understand this think about it, I know the functional point I know this point, I also know the slope. If the slope is like this the function is going to go like this.

If the slope was like this at least locally it is going to go like this, but it is not enough to know the slope you have to know all the second derivative whether it is curving and third derivative and all the derivatives at this point x, that is it is not just the slope at this point. You have to know the slope here; you have to know the curvature here, if I know the third derivative here and all derivatives here. So, slope then the curvature at x equal to a you know the curvature here slope here and all derivatives. If I know all the derivatives here, then I can guess the value of this function here. So, it says the what is it now Taylor series say how do I how do you get that value . So, that is the Taylor series.

(Refer Slide Time: 12:44)

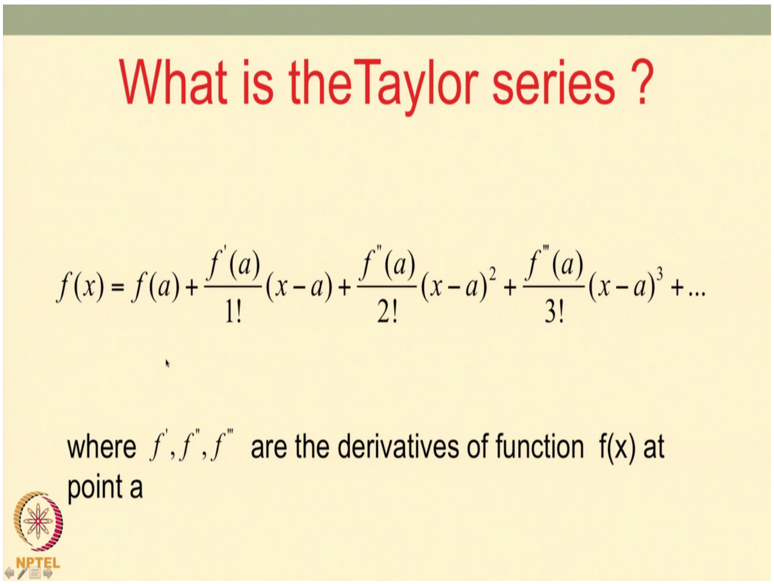


So, it says that if I the functioned at any point x, if I know the point function at a. So, if I know the value of the function at x equal to a, can I know the function at x equal to any value of x . So, the answer is we can.

So, what does the Taylor series say? The Taylor series says we can calculate the function at x if I know the function at a, I have to add to this value of the function something what we have to add? I have to add the first derivative df by dx at x equal to a. This derivative not somewhere this point the derivative the slope at this point x equal to a, times x minus a this distance this minus this. So, this is the point a. So, x minus a is this distance. So, divided by one factorial plus, second derivative that is a curvature at x equal to a times x minus a whole square divided by 2 factorial. So, take the square of the distance and 2 factorial plus the third derivative at x equal to a times x minus a whole cube divided by 3 factorial plus dot dot dot up to infinity.

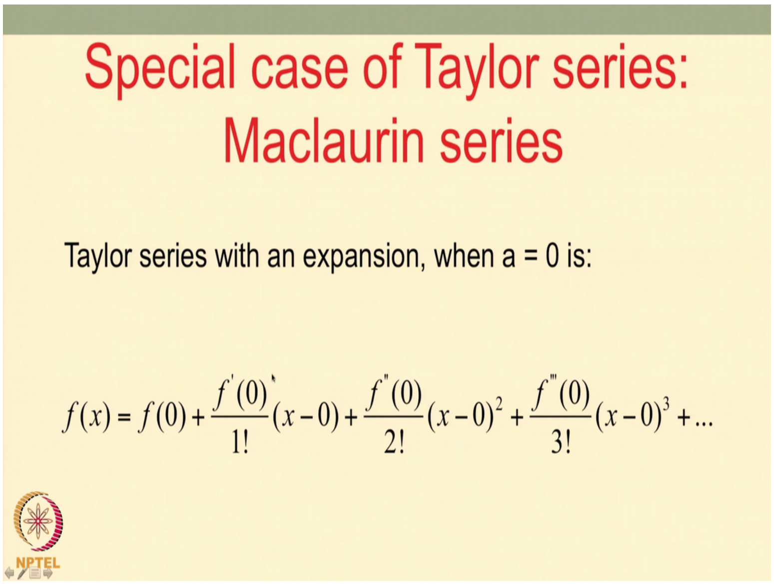
So, if I know the function at a is slope at x equal to a, its second derivative at x equal to a. its third derivative and all derivatives each derivative I multiplied with x minus a to the power n 2 n th derivative, and divided by n factorial in a sum this way, I would get the function at this point. So, sometimes x minus a could be negative, then this will be a minus and so on and so forth. Second derivative first derivative could be negative, second derivative could be whatever be the value appropriately. So, depending on all that you would get this answer, but this is a formula that can be used to know the function if I know the function at a. So, what does the Taylor series say?

(Refer Slide Time: 15:03)



The Taylor series says that, f of x the function at x can be obtained. If I know the function at a to that I add f prime a divided by one factorial times x minus a, that is first derivatives times the difference plus second derivative f double prime a second derivative evaluated at a divided by 2 factorial times x minus a square third derivative divided by 3 factorial times x minus a cube and so on and so forth where f prime, f double prime, f triple prime or at the derivatives of function at f of x at point a. So, if I know all derivatives at a, I can use this and obtain this the I could use.

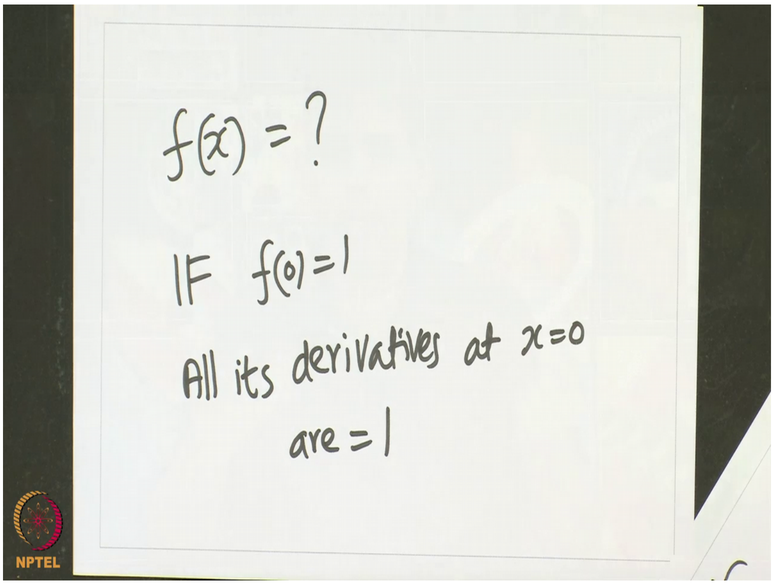
(Refer Slide Time: 15:54)



Now I could use A as 0 So, I instead of a as I could say this would 0 then this would simplify.

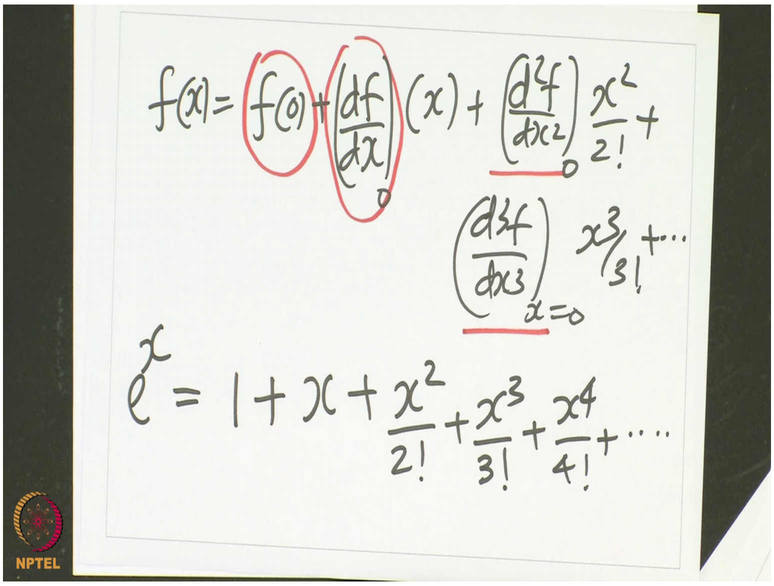
Of course f of x is f of 0 plus f prime the first derivative is 0 by 1 factorial times x second derivative is 0 divided by 2 factorial times x square third derivative at 0, divided by 3 factorial times x cube. So, this is an expansion at a equal to 0 called the Mclaurin series. So, one can use this. Now if I know this how is it useful? For example, the c power x that we learnt or any function sine of x, these are expansions like this. So, let us first consider some function. So, think of a function we have to know what all things we have to know we have to know the value of the function and all its derivatives.

(Refer Slide Time: 16:53)



So, let us think about some functions we want to calculate f of x what would be that function if, what is simplest thing we can imagine. You can imagine that the function at 0 is 1, and all its derivatives at x equal 0 is also 1. All these derivatives are equal to 1. So, this is something which we can start imagining, you know the function. So, for the simplicity let us take the function is 1 and all these derivatives are also one if you assume this, what would we get.

(Refer Slide Time: 17:51)

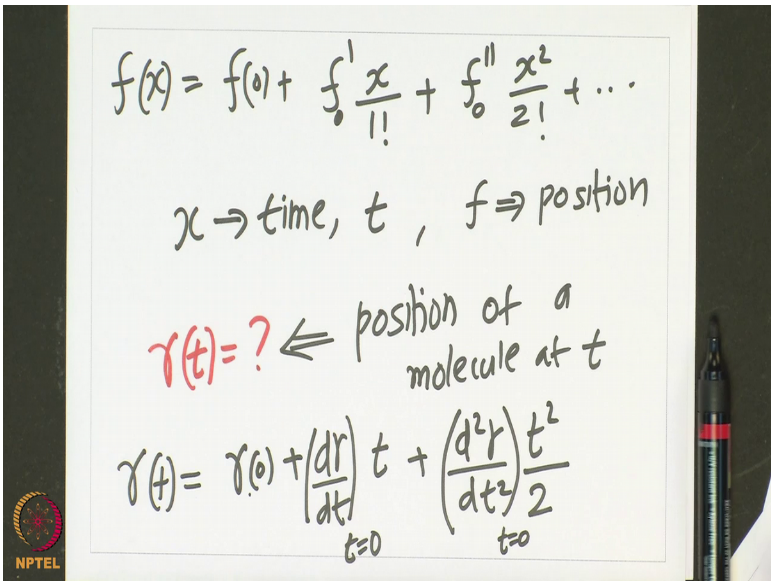


So, let us see what we want what we want we want the function f of x the Taylor series says f of x is f at 0 plus df by dx at 0 times x plus d square f by dx square at 0 times x square by 2 factorial, plus d cube f by dx cube at x equal to 0 x cube by 3 factorial plus infinitely infinite dot dot dot dot.

So, if I do the if I ask the simplest assumption is let us this is to be assumed to be 1. So, I will put here 1, this derivative let us assume to be 1, this is derivative is also 1, this derivative is also 1. So, let us assume all derivatives are 1 then what do we get we will get? 1 plus x plus x square by 2 factorial plus x cube divided by 3 factorial plus x power 4 by 4 factorial plus dot dot dot what is this? This is nothing, but e power x . So, e power x is nothing, but a special function.

So, an interesting function whose value and its derivatives are equal all equal to 1 at x equal to 0 right. It is all the relatives and the value the function itself is same as its derivative, and this would immediately lead to e power x. we have we can have many other application. So, let us think about if we want to know the position. So, what let us write again once more?

(Refer Slide Time: 19:38)



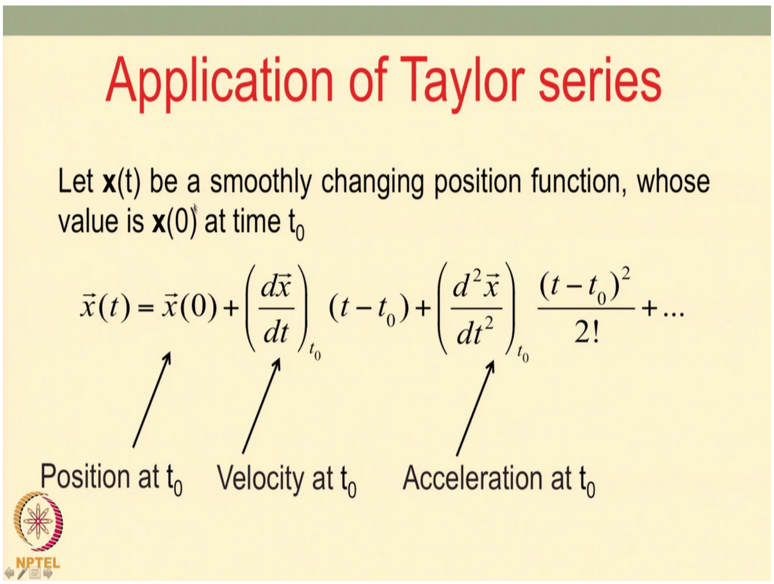
What is Taylor series it says f of x, if I know f 0 and I know the first derivative f prime x by one factorial plus f double prime evaluated at 0.So, this is evaluated at 0 evaluated at 0 x square by 2 factorial plus dot dot dot. So, let us take here x as time. So, I would represent t. So, let us say what we want? We want to know the position of a particle we want to some many things are moving. So, if you want to know the position of a particle at any time t. So, let us write r of t this is what I want to know. I want to know what is r of what is r of t? Position of a molecule in a cell or whatever you not in a cell.

Specifically wherever it be position of a molecule at any time t. If I want to know this I would substitute f is equal to r. So, x is time f is position. So, then if I want to know this let me write r of t is r at 0 if I know the initial position at time is equal to 0, plus the first derivative which is dr by dt what is dr by dt? Is nothing, but velocity at time is equal to 0 this is called initial velocity time. So, x is time plus second derivative d square r by dt square t square by 2 factorial which is nothing, but 2. So, if I use this. So, if I know the initial position and initial velocity and the acceleration at t at this time t equal to 0.

I can get this if I assume all derivatives are 0, its just this you can see if I can do an approximation. So, what do if I just take any Taylor series, if I just assume that. So, if I consider this if I assume x is very close to a, I can neglect all other points. So, it can be approximated if I neglect if I assume x is very close to a then higher order terms can be neglected, if I assume there is x minus a whole power n is very small that is one way, but this is a way of getting position. So, think about this this will turn out to be Newton's equations. So, Newton if you assume that acceleration is a constant and all derivatives beyond third derivatives fourth derivatives etcetera as 0.

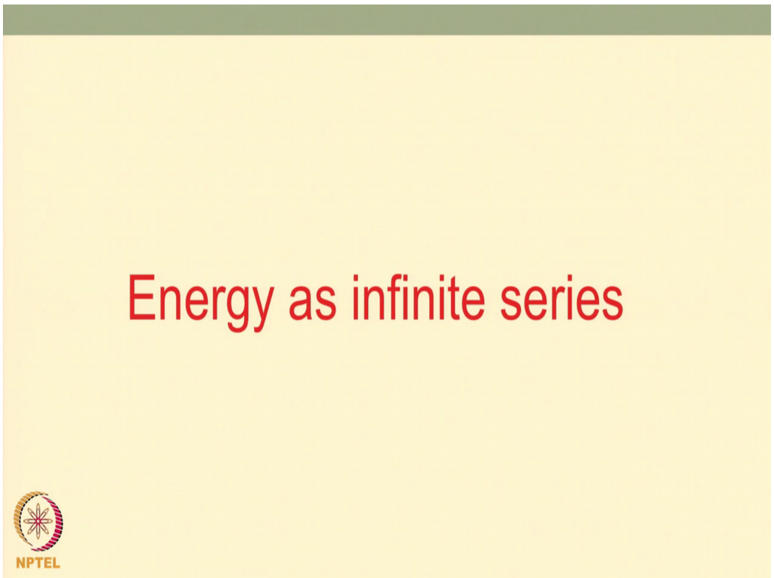
Then we will get this position expansion we will turn out to be Newton's equation. So, let us see here here x is basically the position.

(Refer Slide Time: 23:03)



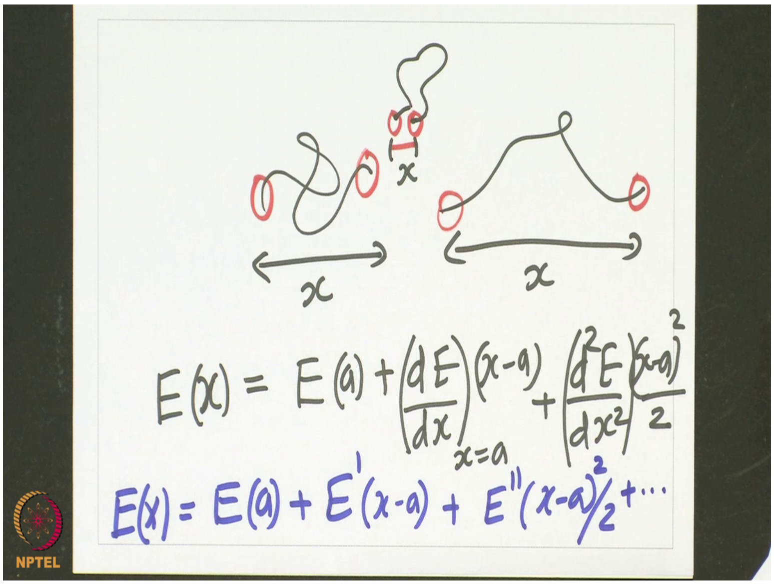
So, x of t be a smoothly changing position function, whose value at x equal 0 is at time equal to 0 if we know. X at any time t can be written as position at t equal to 0 velocity and acceleration. You see this will turn out to be the newtons equation that we all learned in school. So, this is one can using this idea from mathematics, newtons equation will naturally emerge. The only assumption here is if you assume a higher beyond acceleration all derivatives are 0, then this will be precisely the newtons equation. So, the position at any point just emerges from this simple mathematical idea. Can we use this for some other function? So, of course, we can use.

(Refer Slide Time: 23:59)



We can use energy as infinite series. So, let us think about it, what we want? We want to know the energy of a molecule. So, let us say we want to know we have some molecule and this molecule these 2 endpoints are important let us say.

(Refer Slide Time: 24:13)



So, this distance between these 2 endpoints let me call x is this distance between these 2 points. So, energy of the molecule if those 2 points are x distance apart. What does the energy of this molecules? So, this molecule which is could be a protein molecule; this protein molecule could be either like this or it could have some other conformation were maybe like this is this expanded it is stretched and it could be this conformation.

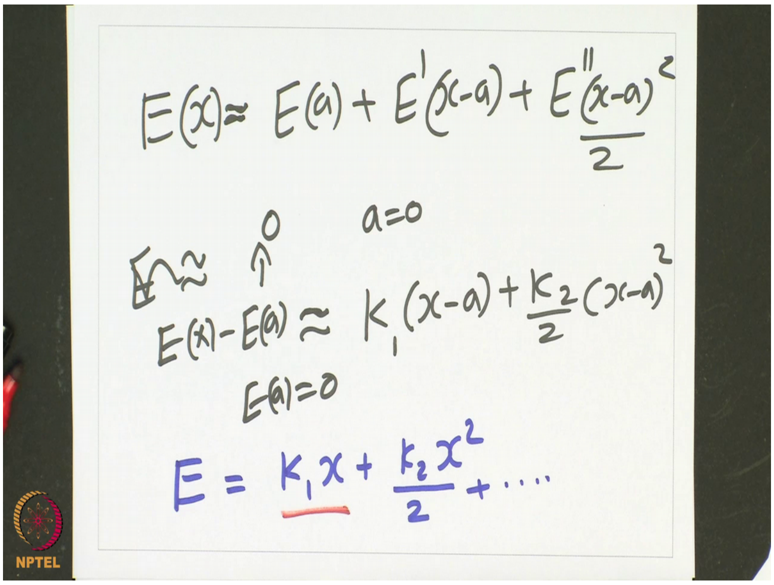
So, in this conformation the distance between these 2 points is very large. So, here x is small here x is very large. So, you could have many other conformation, you could have a conformation where is like this let us let me draw like that is something like this, where those 2 points are very close. So, this x is very small. So, here the x is the distance between these 2 points is they are very close. So, the here these 2 ends are very close here this is some end is some distance upon here it is far away. So, what is the energy of this molecule for a different values of x. So, that is the question that we want.

So, the Taylor series would say that if I know the energy at some other point, some any point x equal to a, some distance if I know the energy at one of these x values, if I know energy for this x value if this configuration energy if we know we can calculate the configuration energy for any other x by calculating the derivative of this dE by dx, at x equal to a times x minus a plus d square E by dx square x minus a whole square by 2 right. So, let me rewrite this, little bit more carefully here. So, if I rewrite this energy at any point x can be written as energy at some energy of some configuration a.

So, energy of the configuration having distance x is energy of this configuration plus derivative of energy e prime means dE by dx times x minus a, plus E double prime second derivative of energy times x minus a divided by 2, x minus a square divided by 2. So, if I know this this is plus dot dot dot. So, if I assume x is very close to a, I can neglect all x minus a cube and x minus a power 4 etcetera will be very small compared to x minus a. So, I can neglect it.

So, again write approximately. So, I can write the following that.

(Refer Slide Time: 27:40)

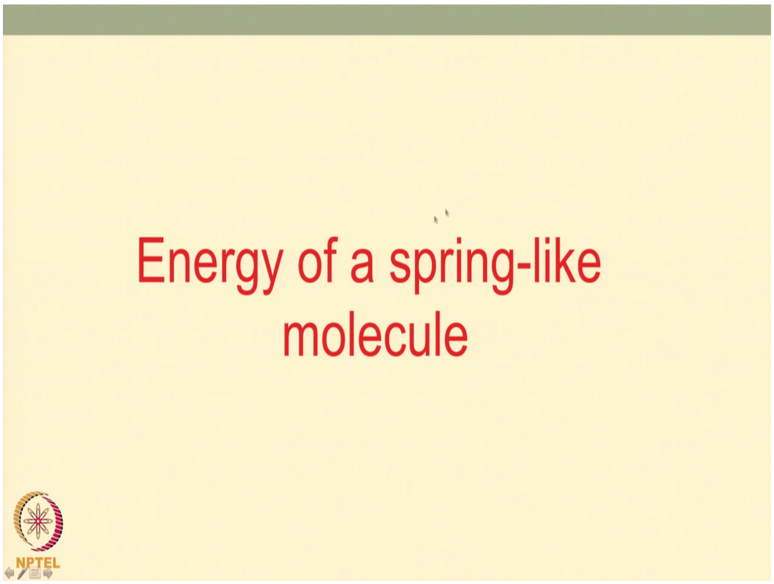


So, what do I can write I can right E at x is E at a, plus derivative E prime x minus a plus E double prime x minus a whole square by 2. So, if I write this is if I plus this is approximately equal to because I neglect higher order terms.

So, approximately the energy can be written as. So, I can take this way and write Ex minus a. So, that is I can write E of x minus E of a this is the change in energy approximately equal to E prime first derivative. First derivative is some constant let me call it k 1 into x minus a plus k 2 by 2 into x minus a whole square. So, if I a if I assume energy at of this is 0 and a is 0, if I take a equal to 0 and e of a equal to 0.So, if I do that if I assume E of a 0, I can write the energy of the delta E as k 1 x plus k 2 x square by 2. So, this is essentially like approximate form of energy plus higher or plus in princi in principle all infinite terms.

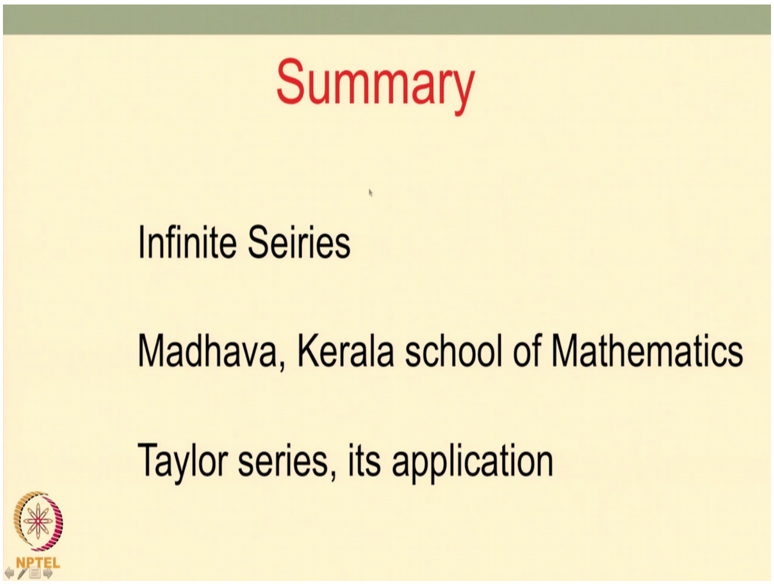
Like this I could write if I know this k one and k 2, I can calculate this energy. So, if I just take a spring like molecule.

(Refer Slide Time: 29:24)



So, if the energy of a spring like molecule, spring has a symmetry that if I compress or expand the energy has to be the same. If I have some symmetry like this I can say that the first derivative will be 0. So, if I assume if I figure out that the first derivative is 0 the energy will be essentially some constant times x square by 2 liken half k x square. So, this is how the half k x square comes, but this kind of expansion is very useful for calculating energy of many proteins and we will use this idea later, many contexts energy can be written as the expansion of functions like this. So, to stop and to summarize what we learned we learned.

(Refer Slide Time: 30:09)



The idea of infinite series we learned Madhava and Kerelas school of mathematics how they shattered it we learned about Taylor series in its applications and we talked about applications for a position as a function of time application for energy, you get a looting of concentration into some point x is, how can we calculate the concentration of somewhere as a Taylor series can we do that I urged think about it. So, the idea of this lecture is can we calculate our favourite function at some bar index see if I know the function at some other point and all is derivatives. This idea will be used very often at in various places think about this, and this is extremely useful with this I will stop the todays lecture bye.

Bye.