Introduction to Dynamical Models in Biology

Dr. Biplab Bose
Associate Professor
Department of Biosciences & Bioengineering
Indian Institute of Technology, Guwahati

Lecture 5

Numerical solution of ODE - 1

Hello! Welcome to module 5, week 1 of our course on introduction to dynamical models in biology. In last two modules, two or three modules rather, we have discussed how to make ordinary differential equation based mathematical model to understand dynamics in a biological problem. Remember the key issue in case of ODE based model is that you write one or more than one ordinary differential equation representing rates of the processes involved and then you integrate those ODEs to generate a function which gives you option to analyze the system and get answer to your questions.

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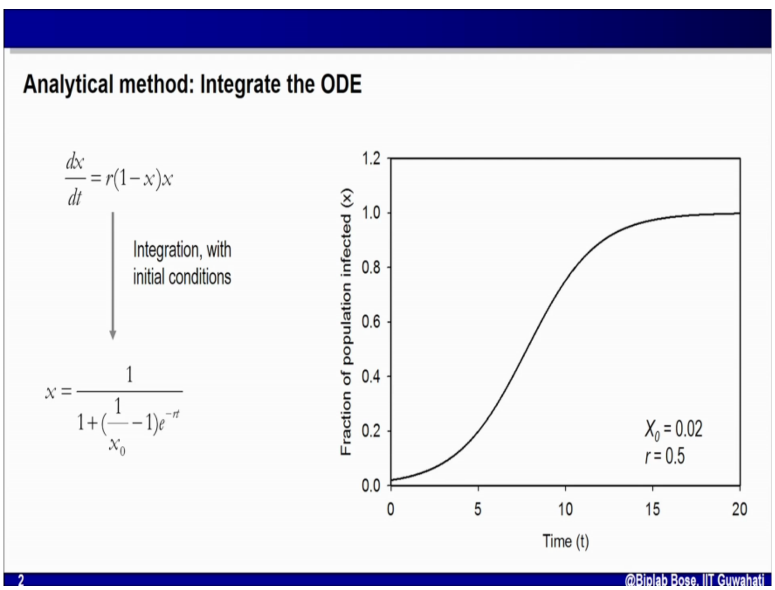

For example, if you remember the question of the spread of infectious disease when we are trying to model that is one, we wrote an ODE, we representing the rate of change in fraction of population infected that was $dx/dt = r(1-x)x$. Now this is the ODE 'Ordinary Differential Equation'. We integrate this ODE with initial conditions given to us and we got a function for x. So this x is a function of time. So by integration we got this. Now if we replace the value of x_0 in this function and the value of r with a numerical value then we can know what will be the fraction of population infected at a particular time t or rather if we take different values of t for a fixed value of x_0 and r then we can draw a graph like this one as shown here. Now this we have discussed for two three problems for example growth of population, logistic growth of population like that.

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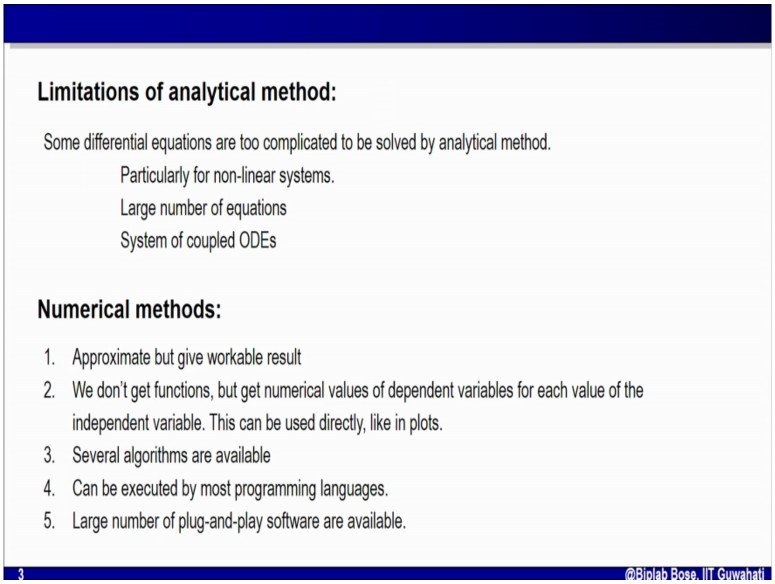

Now this procedure, this technique has one problem. Here what we are doing, we are integrating an ordinary differential equation using symbolic math. This method is called analytical method of solving the problem. The problem is for many ordinary differential equation particularly which are nonlinear ordinary differential equation it is usually very complicated to solve those equation using symbolic mathematics or rather analytical, the way we have done it earlier. In many cases the number of ODEs in our problem will be very large. In those cases it becomes very complicated to solve them and secondly it's symbolical and particularly this is true when your system of ODEs actually coupled ODE and that will happen very frequently in biological problem that we deal with.

So in all these cases usually either it's very complicated or we don't know right now the method to solve these equations, so how will you approach this problem? If we don't know the method or if the method is very complicated to solve then how we will solve the system of ODEs. Thankfully there is a numerical method. Numerical methods are more very useful because we can implement them to computers so actually you can ask computers, even your desktop computers to solve a particular set of ordinary differential equation and give us the answer. In these modules we will discuss about the general aspect, the basic features of these type of numerical solution system or rather algorithms for numerical solutions.

Now before we go into that, let us look into the basic aspects of numerical methods. The first issue is numerical methods are actually not exact methods. They are approximate and the approximation is such that they are workable. So whenever you are using a numerical solution for your ordinary differential equation using a computer you have to remember that the solution that you are getting is approximate one and we have to take care so that the approximation is as close as to the real solution. In these algorithms we don't actually get a function, the way we got in case of integration. By integrating analytically or symbolically you have got a function for the dependent variable but when you are doing numerical solution, you won't get a function rather you will get a data for change in the value, different values of the dependent variable with different value of independent value.

For example, if we numerically solve ODE for the spread of infectious model we will have data for each time point then we will have data for x. So we get numerical data. Now that numerical data can be used in various ways. You can make a plot with time in horizontal axis whereas the X, the fraction of population which is infected in vertical axis. By doing so you can visualize how x will change with time and in fact that's what you want so numerical solutions actually gives you direct data which maybe approximate slightly it gives you direct visualization you can have so how dependent variable is changing with independent variable. Thankfully there are many algorithms for numerical solutions are available.

Some are very good for particular type of system whereas others are better for other types of ordinary differential equations. And in fact most of these algorithms can be implemented by most of the common computing brand that we use whether it is C, FORTRAN or if you want to use MATLAB, you can actually write few lines of code. These languages have library functions made by somebody else which you can use for solving your ODE numerically. At the other side actually there are many plug and play software's where you do not need any knowledge of programming. You can simply write down the equations for the ODE and ask it to solve. So numerical solutions for ordinary differential equations are very advantageous because we already have readymade tools for that.

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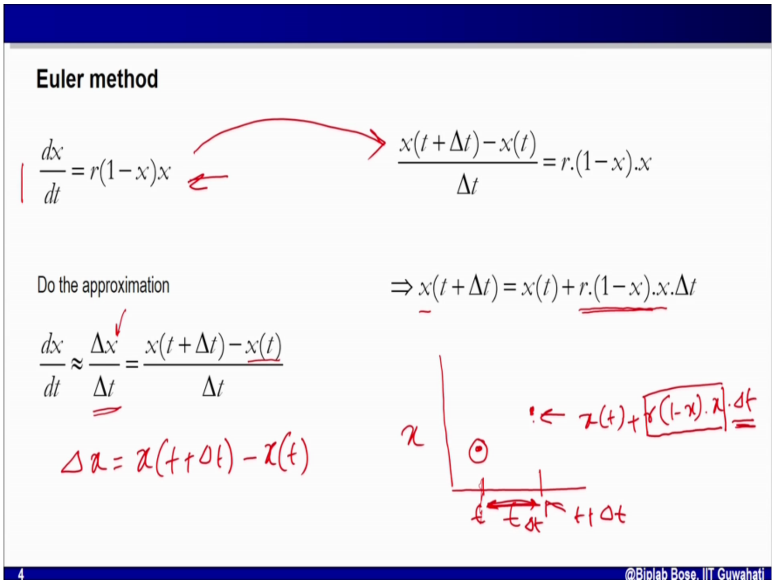

So let us look into the basic aspects of numerical solution of ordinary differential equations. There are many algorithms as I said earlier for solving a system of ODE or a single ODE numerically. I will start discussion with Euler's method because it is the simplest method to understand. Remember Euler's method has exchange sheet mathematical background. I won't go into that exhaustive math but I will try to convey to you the basic message of this Euler's method, the basic issues of this method intuitivly. So let's start with the example. We have a differential equation here representing that rate of spread of infectious disease, $dx/dt = r(1-x)x$. You have seen this equation earlier.

Now I want to solve this numerically using Euler's method. So the first important thing that we have to understand, dx/dt is actually where changing x and time are infinitely very small. I can approximate it, consider it, there is a finite change in time that is Δt and there is finite change in 'x', Δx so dx/dt with approximation obviously is equivalent to Δx/Δt. What is Δx? Δx is value of $x(t+\Delta t) - x(t)$. so Δx is nothing but value of $x(t+\Delta t) - x(t)$. So Δx/Δt is $x(t+\Delta t) - x(t)$ divided by changing time Δt. Once we have this one then we can rewrite this first equation that ODE in this form. So dx/dt is equivalent to $x(t+\Delta t) - x(t)/\Delta t = r(1-x)x$. We are getting this one from this first equation ODE.

If I rearrange this term so that I keep $x(t+\Delta t)$ only at the left hand side and everything on the right hand side then I get this one, $x(t+\Delta t)-x(t)/\Delta t=r(1-x)x.$ This has come mainly from the ODE into Δt. that means if I am, I will show you graphically this is time ‘t’, ‘x’ is varying here. At suppose time ‘t’, ‘x’ is here and after time Δt, this is Δt. So this is nothing but t+Δt . I will be somewhere here and this value is ‘x’ at time ‘t’. this is the $x(t)+r(1-x).x.\Delta t$. Δt is this distance. The change in time. We call it the time step. so Δt so the time state so remember r(1-x) and ‘x’ is coming from differential equation that you have written. So what is happening here you start with ‘t’ at a particular time then you increment time by small Δt and then you calculate the value of x(t+ Δt). Once you have calculated this one, you can take another time step of Δt and again calculate the value of ‘x’ at that so in this iterative way you can keep on going calculating value of ‘x’ as I change the value of ‘t’ with Δt.

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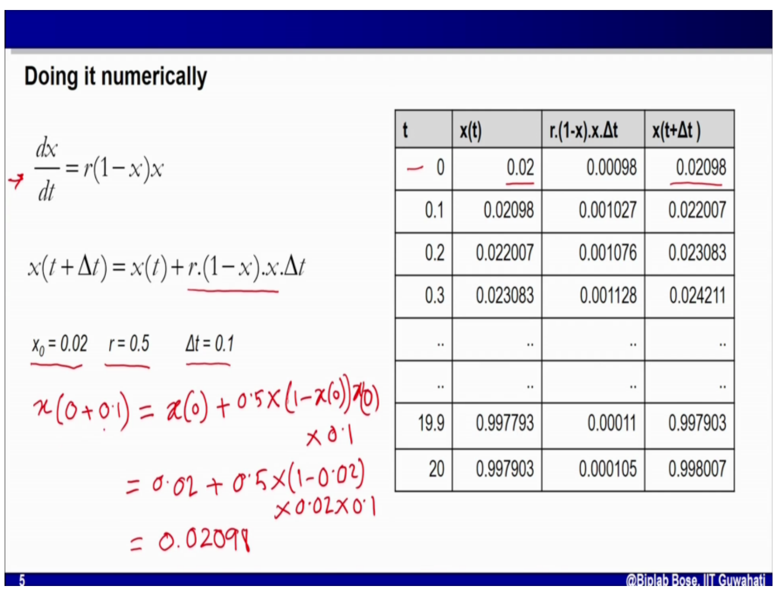

Now let us try this numerically. We will take the same example of spread of infectious diseases so our ODE is as usual as the last one $dx/dt=r(1-x).x$ and the formulation from Euler’s method that we have got is $x(t+\Delta t)=x(t)$ into the function that is present in the ODE into Δt. If you remember to solve your initial condition so $X_0(t)$=0.02. R is 0.5 and Δt is the steps of time that will take is 0.1. So now at time ‘t’, x=0.02. ‘x’ at next time point that is 0 + 0.1=x(0) + R is $0.5*(1-x(0))*x(0)*¿$ Δt is 0.1. If we put this one, x(0) is

$0.02+0.5(1-0.02)*0.02*0.1$. 0.1 is for Δt, the increment in time. I have already done the calculation and it comes to 0.02098.

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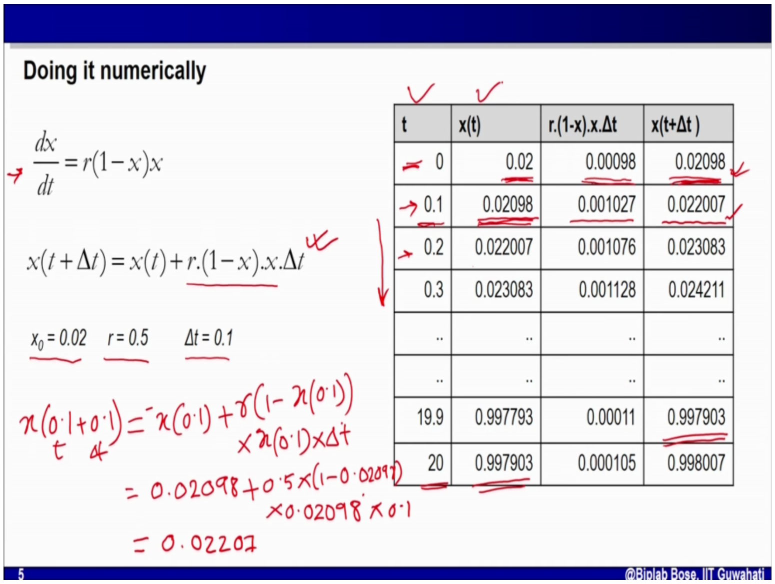

I have made a table here, at time t=0 , your value of ‘x’ is 0.02 and you get by this calculation the value of x(0)+0.1 will be 0.02098. Now that is the value of x(0+ Δt). That means my clock has changed by 0.1. So you calculate what will happen at that point. At point 1 our value is 0.02098. This value is coming from this one. Now again if I increment time by 0.1 that is Δt, I had to calculate what will happen at x(0.1+0.1) so this time, this is time and this is Δt. Again I will use the same formula which is this one we are getting for Euler’s method so I have to take value of x(0.1)+r(1-x(0.1)).x(0.1).Δt. So I know x(0.1) is 0.02098 + R is $0.5(1-0.02098).(0.02098)*0.1$ is Δt. This will be equal to as I have calculated earlier is 0.02207. That value is shown here.

If you see this table I started with time $t=0$. It is given time $t=0$ value of $x=0.02$. I calculate the value of $r(1-x).x.\Delta t$. This value is this one so I increment x by this value and I get value of $x(0+0.1)$ time point as this one, 0.02098. So that means I write the same value again, time is 0.1, value of x is 0.02098. Again I calculate this one which is $r(1-x).x.\Delta t$. I sum these values with value of x and I get the value of $x(0.1+0.1)$. Time point is 0.2 time point as 0.022007. So I write the same value here. So at 0.02 I have value of x as 0.022007. In this way I can keep on calculating the value of x at different time points with increment of 0.1. As you can see in the table, initially the time is 0 then $0+0.1$ is 0.1 then $+¿$ 0.1 is 0.2 and then + 0.1 is 0.3. In this way I have done up to time 20 and the value of x at time 20 is obtained here at 19.9 times 10 is 99.7903.

I have these two data, $r\, vs\, x$. I can easily take them and make a plot and then make a graph showing change in x with respective time. The interesting thing is that the Euler's' method is very easy and for one or two equations ODEs you can actually implement it using Microsoft excel.

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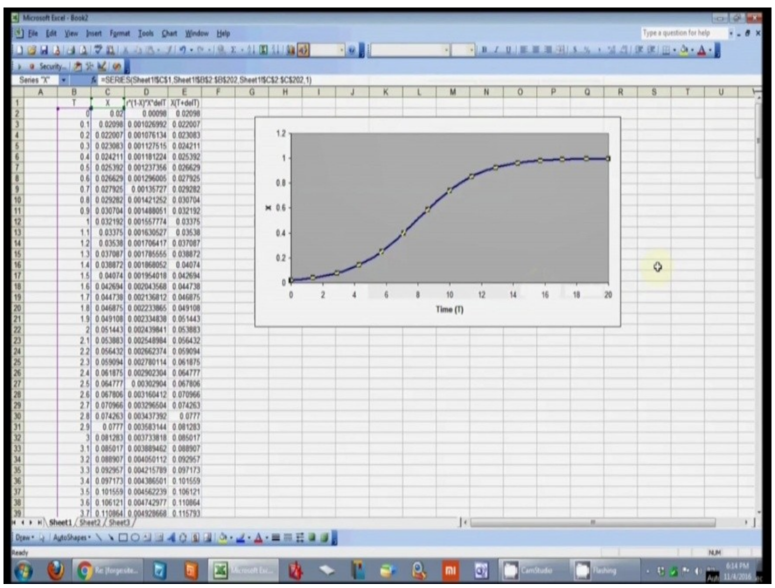

So in here I will show you how I have implemented it in MS excel. I will strongly advise you to do it yourself using Microsoft office tool that you have. You must have got Microsoft excel with you and try this. First I will put the header. First one is t time, next column is for x at particular value of time then I calculate $r(1-x).x$ in the next column $¿\Delta T$ t there is an increment in time. Then adjust the size of the cell then you have new value of $\frac{t+\Delta t}{x¿}$). let us see the value. This is the header. First time point is 0, at that time point our value of x was 0.02 so now I use the formula of excel to calculate the value of $r(1-x).x.\Delta t$. I is given as 0.5 into 1 minus this one.

See how I am choosing C2 as value for x, into $C2 ¿(\Delta t)$ =0.1 so now this is my increment that is $0.5(1-C2)$ because C2 is holding the value of x at that moment into C2 $¿(0.1)$. The next cell we increment x by D2 so C2 + D2 that is the incremented value of x. This is the value of $x(0+\Delta t)$. In this way we have calculated new value so we increase the time, time should be incremented by 0.1 state so this is value in the previous cell plus 0.1, so I get 0.1. Now the value of x for this will be coming from E2 cell because that is the value we calculated so you will make that one equal to E2 so that is the value of x that we calculated earlier.

Now I have to calculate the increment so I simply pull down, apply the same formula which is present in the D2 cell so you note down that now it is $0.5(1-C3)*(C3)*(0.1)$. Similarly I pull down and apply the formula present on E2 to E3 which is now C3 + D3. So that is the value of x and my time point is 0.1 + 0.1. So this way we have calculated the value of x increment. Now all the formulas are ready and I have extended and applied to all the cells till I reach time point 20. So we have got 20 so at 20 time steps as you can see the value of x is 0.9973 so we choose t and x column, these are the values we require and these are the plot function to plot. From X axis we mark it as time, Y axis is the value of x so we mark it as X and finish it. We can remove this legend and deadlines; adjust the skill because we require only about 20. Now I thicken the size of the line a bit so that it looks better and that's all. Now you have the behavior of x versus time as calculated using the ODE and solved by the Euler's method and it looks almost similar to that what we have got earlier using the analytical methods.

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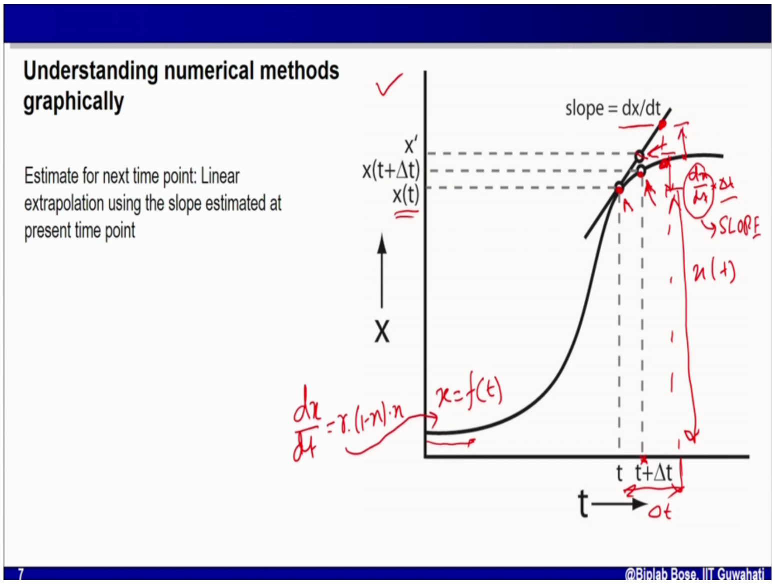

Let us look into the Euler's method in a graphical way. Look at this graph given here. Suppose at time, t we are at this $x(t)$ point. At this $x(t)$ point, this curve shown here is essentially function of x as a function of time t and we have got it from a differential equation. We have differential equation which was $r(1-x).x$ from integrating that we have got this function and this is the function. At time t we are at this point so the value of x at time T is $x(t)$. Now we increment the clock by Δt so our time point is $t+\Delta t$ and we want to know the value of x at that point. So using the exact solution the value will be this one, $x(t+\Delta t)$ but what we do in Euler's method is that at this point, at time T we are drawing straight line having a slope which is equal to dx/dt and we are extending this line till we meet $t+\Delta t$ position so we get this line.

We take this point as the value of x at $t+\Delta t$ so what we are doing initial the value of x is this one, this is $x(t)$. We are incrementing this one by $\frac{dx}{dt}*\Delta t$. So this is the increment. So this is first part which is actually nothing but slope and the second part is the Δt, increment in time. But as you can notice, there is a gap between this calculated one and the real one. Now if I increase Δt, if I make Δt bigger, suppose I take this portion, this whole thing as Δt, the bigger Δt then by my method I will have the new value of x here whereas the real value is actually here so you can see at every stage what we are doing as we are incrementing time by Δt and using the slope at a particular time point to get the new value of x through extra collation we are getting an error estimate. This is our error estimate. This error estimate can be reduced if we can make Δt small.

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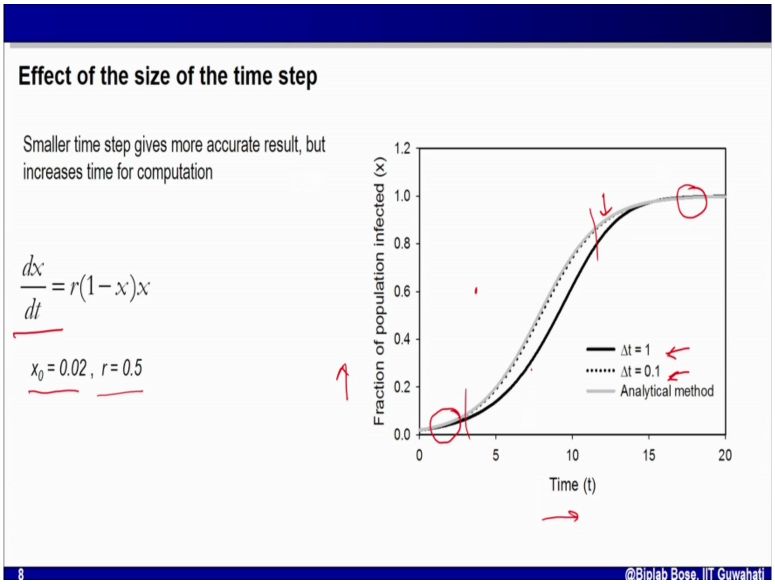

Now let us see the effect of this one. It's the same ODE for spread of infectious disease; the initial value is same as earlier 0.02. r is 0.5 and I have plotted different data. In your horizontal axis you have time t and your vertical axis has x, the grey line as you can see here is the exact solution obtained by symbolic mathematics of analytical method. We have done it earlier. I have done the numerical simulation using Euler's method using Δt as 1 and Δt as 0.1 so one Δt is bigger than the other. The black line shows when Δt is 0.1. My result from Euler's method whereas the dotted line shows the result of Euler's method when Δt is 0.1. So as you can see initially both the analytical method and both the numerical method are giving similar result.

At the end also we have all these three matching together but in between here and here you can see there is a difference between different method. When Δt is 0.1 it's almost same as analytical method but when you are taking bigger Δt, we are getting an erroneous result and that is shown by this black line. So as I said in the previous case that the correctness, the approximation, the goodness of approximation will depend upon the Δt we are taking. The smaller the t, the better the result we get and the errors will be less.

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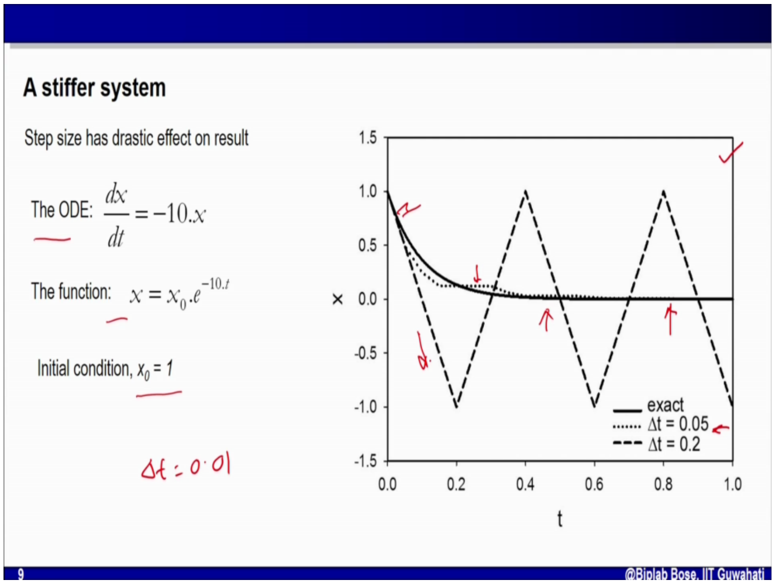

Let us take another extreme example to understand this plot. In this case the ODE is very simple. ODE is $\frac{dx}{dt} = -10x$ so it's almost like exponential. If you do integration with initial condition you get this function $x = x_0 . e^{-10.t}$. x_0 is the initial value of x when $t = 0$, so let us solve it considering x_0 ¿1 . Look at the graph. The black line is the exact analytical solution. I have not shown here but if you take Δt for Euler's method for solving this system, Δt = 0.01, you will get a solution which will be very close, almost exactly same as the analytical solution shown in the black line. If you take Δt slightly bigger, 0.05 which is shown in the dotted line here, you can see for most of the part here and here, it is similar to the analytical method but in some portion it is deviating and we have some error.

But this deviation is absurdly very high when you take Δt =0.2 then you can see this bigger line; the value of x is almost rhythmically varying with time which is absurdly wrong. So what I want to show you here is Euler's method very simple numerical method which you can implement in Microsoft excel for small system for one or two ordinary differential equation but you have to keep in mind that this system, this algorithm is very sensitive to what is the step size or the increment size for time that you have taken that is Δt . if you take very large Δt then you will have erroneous result. If you take small Δt your result will be very good but you have to remember that your computation time will also increase.

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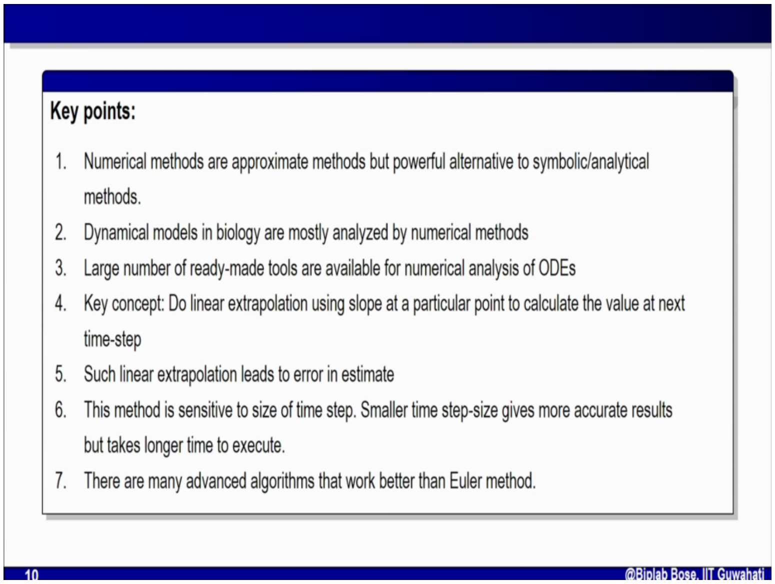

So to jot down the key points, what we have discussed in this module is that, analytical method or symbolic method that we have used to integrate an ordinary differential equation to get a function for our model is useful but becomes difficult to use when number of ordinary differential equation increases or we have a system of ordinary differential equation or you have a large number of nonlinear ordinary differential equation. In those cases, numerical method, numerical algorithms for solving ordinary differential equations are very powerful. Those numerical algorithms will give you approximate answers but those answers are coactive.

We have to remember that in biological modeling we have large number of variable so we have large number of ordinary differential equation and for most of the cases we will not be able to analytically or symbolically solve them and we have to rely on these numerical algorithms. There are many numerical algorithms available. I have discussed the basic one, the Euler's method to understand what is going on behind these numerical algorithms. We have seen that this is very easy to implement, even on Microsoft excel we can implement this one. We have observed that this method is sensitive to the step size or the increment in time that you get that is Δt . If you take very large Δt , we will have error in your calculation. If you take small Δt , your computation time will increase.

There are many other algorithms for numerical solution of ODE. We will discuss them in the next video, in the next module. Here we should keep in mind that numerical methods are very popular because in most of the languages, computational languages that are available with us, from C to FORTRAN, to higher level things like MATLAB, we already have library functions to implement this algorithm. At the same time if you are not habituated with programming, there are some plug and play software's, large number of them which you can use to solve your ODE, a system of ODE using numerical method. So as a whole numerical methods are very powerful tool and bread and butter in ordinary differential equation based modeling for biological system. Thank you for listening. See you in the next module.