

Mathematics for Chemistry
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Module – 05

Lecture – 21

Differential equations, order, 1st order ODEs, separation of variables

So today we will start module 5 and module 5 is the first of 4 modules on differential equations. So, the second part of this course will entirely be about differential equations. In module 5 we will focus on first order differential equation. So, there will be 5 lectures each about half an hour long and the first lecture, I will introduce differential equations, I will introduce the order of a differential equation, I will introduce first order differential equations and the basic techniques of separation of variables to solve them. In the second lecture I will be talking about exact differentials and how they can be used to solve first order differential equations. In the third lecture we will talk about integrating factors. In the 4th lecture I will go to a system of first order differential equations and where you can use matrix methods to solve them and then finally, we will end with some practice problems.

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Types of Differential Equations

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Mathematical equation involving derivatives

<p>Ordinary differential equations (ODEs) One independent variable ordinary derivative $\frac{dy}{dx} = 3x^2 + 2y$ Examples: Chemical kinetics $\frac{dC(t)}{dt} = -kC(t)$</p>	<p>Partial Differential Equations (PDEs) ↓ Depend on more than one variable - Partial derivatives $\frac{\partial^2 y}{\partial x^2} = c^2 \frac{\partial^2 y}{\partial t^2}$ T.D. Schrödinger Equation for 1 particle $-\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi = i\hbar \frac{\partial \psi}{\partial t}$</p>
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So, let us get started in this. So, I will start with differential equations now what are the types of differential equations. So, a differential equation is typically an equation that

involves derivative. So, differential equation is a mathematical equation involving derivatives. So, now, the types of differential equation, broadly you can think of what are called ordinary differential equations also called as ODEs and there are partial differential equations this is PDEs and really the most important thing about partial differential equations is that this has dependence on multiple variables. So, it has quantities that depend on more than one variable able this involves partial derivatives for example, you can have a partial differential equation that looks like $\frac{d^2 y}{dx^2} = c^2 \frac{d^2 y}{dt^2}$. So, this is an example of a partial differential equation and also partial derivatives ordinary differential equations in this case there is only one independent variable and you only have ordinary derivatives. So, for example, you might have $\frac{dy}{dx} = 3x^2 + 2y$ this is an ordinary differential equation.

Now, in this part of the course I will be talking only about ordinary differential equations I will not be talking about partial differential equations and, but occasionally if you have to do with partial differential equations and lot of the techniques that you learn in ordinary differential equations can actually be applied in those cases also now what are the examples of differential equations where do you see them. So, the most common examples I mean you see them everywhere in chemistry, but one example where you are used to seeing differential equations is when you write kinetics in chemical kinetics. So, you write something like $\frac{dc}{dt}$ you might write it as $k \cdot c$ for a first order kinetics, etcetera or you might write or if you have multiple species then you write c_1 , c_2 and so on.

Now c is a function of t , this is a concentration which is a function of t and I mean if you could have something that is looks like $-k \cdot c$ of t which is a first order decay other example the classic example of partial derivatives, this equation incidentally this partial derivative differential equation is a form of what is called the wave equation, but the other very common partial derivatives that you are used to seeing it is the time dependent Schrodinger equation in quantum mechanics time dependent or even the time independent Schrodinger equation. So, that typically looks like $-\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi = i \hbar \frac{d\psi}{dt}$ this is for a single particle. So, you will have $\nabla^2 \psi + V \psi = i \hbar \frac{d\psi}{dt}$.

So, this is a partial differential equation ψ you are in this case, ψ is the variable ψ is a function of both r and t r is the spatial coordinate a 3 dimensional spatial coordinate and time and I am not showing the dependences and similarly V is also a function of r . So, this is a time dependent Schrodinger equation for a single particle and there are many such equations you can also write the time independent Schrodinger equation I would not bother with doing that here now I will just mention couple of problems that you are used to when you deal with differential equations. So, there are different kinds of problems there is what is known as a boundary value problem where you might have something like your like let us take the example of the Schrodinger equation.

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Boundary value and initial value problems

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T.I Schrodinger Equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E \psi(\vec{r})$$

2nd order D.E. → need boundary conditions

Initial value problem

$$\frac{\partial c(\vec{r}, t)}{\partial t} = D \nabla^2 c(\vec{r}, t)$$

$$c(\vec{r}, 0) = f(\vec{r}) \quad \text{Initial form of } c(\vec{r}, t)$$

Differential Equation ↔ Boundary conditions

So, if you look at the time independent Schrodinger equation. So, this is time independent. So, there is no time. So, the time independent Schrodinger equation is written for a single particle is written as minus \hbar^2 by $2m$ you have a del square ψ plus V times ψ is equal to E which is a constant times ψ . So, V is a function of r ψ is a function of r E is not a function of r .

So, now this problem this is a second order differential equation differential equation and you need solve it. So, this need boundary conditions to solve it. So, you need boundary conditions and we will take examples of lot of these later, but this would be what is called a boundary value problem. So, a differential equation where you give the value of the function at the boundaries would be what is called a boundary value problem now in

now sometimes you get what are called as initial value problems. So, you might get for example, if you have your rate law value problem this I will take the example of what is called the diffusion equation.

So, the diffusion equation says $\frac{dc}{dt}$ is a function of both spatial coordinate and a time coordinate this is $\frac{d^2c}{dr^2}$. So, this is a second order differential equation and often in this equation you prescribe the initial value. So, you say what is c of r at t equal to 0 is some function some function I will just call it f of r . So, this is initial form of c of r this should be c of r t and this is what is called an initial value problem. So, so you can have both boundary value problems initial value problems and essentially differential equation is related with what is called boundary conditions. So, boundary conditions are part of specification of the differential equation and this will be clear when we write down the certain differential equations.

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Ways of writing first order Differential Equations

Order of an ODE = Highest derivative

$$\frac{d^2y}{dx^2} + 2x \frac{dy}{dx} + 3xy = 0$$

↑ 2nd order DE.

1st order DE. ⇒ Highest derivative is 1st derivative

$$\frac{dy}{dx} = f(x, y) \quad f(x, y, \frac{dy}{dx}) = 0$$

ex. $2x(\frac{dy}{dx})^2 + 3y \frac{dy}{dx} + 4x = 0$

$$M(x, y) dx + N(x, y) dy = 0$$

LINEAR D.E. ⇒ Highest algebraic power of dependent variable or any of its derivatives = 1.

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Differential Equations

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Nonlinear DE.

$$\frac{d^2y}{dx^2} + 3xy + 2 \frac{dy}{dx} x^2 = 0$$

$$\frac{dy}{dx} = 3y^2$$

So, what are the ways of writing first order differential equation? So, I will just mention that an order of a differential equation of an ODE let us take an ordinary differential equation is equal to the highest derivative. So, it is a highest derivative that that appears in the equation. So, for example, if you have if you have a in equation that looks like d square y by d x square plus 2 x d y by d x plus 3 x y equal to 0 then this is a second order differential equations. So, first order differential equation implies highest derivative is first derivative.

So, in other words an example, what are the ways in which you can write first order differential equation you might write something like $\frac{dy}{dx}$ is equal to $f(x, y)$ in general some function of x, y , it could be a constant, it could only be dependent on x , it could only be dependent on y , but it is some in general some function of x and y . So, this is one way you could write it, but there are other ways also you can write it you might you might have a differential equation where you do not write it separately like this, you might write it something like I will just write it in this form. So, I will just say some function of x, y and $\frac{dy}{dx}$ equal to 0.

So, this is another way of writing differential equations. So, this is an example of this would be example suppose you have $2x \frac{dy}{dx} + 3y^2 + 4x = 0$. So, this is some function of x, y and y' and that is equal to 0 and notice that even though you are squaring this derivative the highest derivative that appears is 1. So, it is actually a first order differential equation and I just, you can have it in this form also a third way which is often very useful is to actually consider something like this.

So, imagine that you have a ratio of 2 functions and then you multiply it out and you write it in the form. So, you write it as $m(x, y) \frac{dy}{dx} + n(x, y) = 0$. So, I am rewriting the differential equation in this form. So, this is another possibility that you can have. So, you can often rewrite the differential equation in this form. So, basically there are different ways in which you can write the same first order differential equation and you know we will use each of them and we will choose which one is more convenient for our case.

Now, a few more things I want to mention. So, what is a linear differential equation implies highest algebraic power of dependent variable or any of its derivatives equal to 1. So, a linear differential equation means the highest algebraic power of the dependent variable or any of its derivatives is equal to 1. So, for example, you could have a differential equation that looks like let us say $\frac{dy}{dx} + 3xy + 2 \frac{dy}{dx} = x^2$ equal to 0.

So, this is a linear differential equation because each term each term has y raised to 1. So, this has $\frac{dy}{dx}$, this has y this has this is also has $\frac{dy}{dx}$ you could even have a $\frac{d^2y}{dx^2}$ it would still be a linear equation. So, whatever derivative you

have you have no power of a, you have no power that is greater than 1. So, as opposed to, this is a non-linear I will write a non-linear differential equation. So, this for example, you could just have $\frac{dy}{dx}$ equal to $3y^2$. So, now, y^2 is a non-linear term. So, it depends on y to the power 2 greater than 1. So, this is a non-linear differential equation.

So, linear differential equations have either y or its derivative only up to 1 up to the first power. So, these are the kinds of equations that you have and now what do you do with the differential equation you solve it. Now there are different things that you have to keep in mind while solving it now when you solve the differential equation.

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The slide is titled "Implicit and Explicit Solutions" and features the NPTEL logo on the left and a circular logo on the right. Handwritten notes in red ink define the terms:

- D.E.:** $f(x, y, y') = 0$ where $y(x)$ is the dependent variable and x is the independent variable. The derivative is given as $y' = \frac{dy}{dx}$.
- Solution:**
 - Explicit:** $y = g(x)$
 - Implicit:** $f(x, y) = 0$
- Examples:**
 - For the differential equation $\frac{dy}{dx} = \cos x$, the explicit solution is $y = \sin x + C$.
 - For the differential equation $\frac{dy}{dx} = \frac{-y}{xy}$, the implicit solution is $xy + \frac{y^2}{2} = 0$.

So, suppose let us take the; we will consider the case where y of x y is a function of x and this is the y is the dependent variable and x is the independent variable and let us say my differential equation f of x y y prime equal to 0 where y prime equal to $\frac{dy}{dx}$. So, this was one of the ways we could write the differential equation. So, this is the differential equation that we consider.

Now if you consider such a differential equation. So, the solution can be either explicit; that means, y is equal to some I will just say g of x . So, that is an explicit solution. So, so in an explicit solution you right you have your left hand side is y and your right hand side is some function of x . So, when you solve it did you say that this is the solution or

you could also have an implicit solution where you do not actually separately right y equal to something you have some function of x and y equal to 0.

So, an example suppose you have $\frac{dy}{dx}$ equal to $\cos x$ then when you solve this you will write y is equal to $\sin x$ plus some constant this is an explicit solution, on the other hand if you have something like $\frac{dy}{dx}$ is equal to minus y divided by x plus y multiply it out you will write x times $\frac{dy}{dx}$ and then you have plus y times $\frac{dy}{dx}$ and then you have is equal to minus y times $\frac{dx}{dx}$ and you can write the solution by bringing this $\frac{dx}{dx}$ to the left. So, you will have you will have something like $x \frac{dy}{dx} + y \frac{dy}{dx} + y \frac{dy}{dx}$ equal to 0 and what you realize is that this is just d of $x y$ this is just d of $x y$.

So, when you integrate this you can you can show that $x y$ and this is d of y square by 2. So, plus y square by 2 equal to 0, this is an implicit solution. So, you can have both explicit and implicit solutions for differential equations now the other point about differential equations is that you can have general solutions and particular solutions. So, so we already saw here. So, if you look at your differential equation.

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The slide content is as follows:

General Solution, Particular Solution

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$\frac{dy}{dx} = \cos x$ $y = \sin x + C$ → arbitrary constant
 General Solution

$\frac{dy}{dx} = \cos x$ B.C. $y(0) = 0$

$y = \sin x + C$

$0 = \sin 0 + C \Rightarrow C = 0$

Particular solution: $y = \sin x$

If you look at this differential equation, $\frac{dy}{dx}$ is $\cos x$, now you have y equal to $\sin x$ plus a constant. So, I will just write it again. So, $\frac{dy}{dx}$ is equal to $\cos x$ then you say y is equal to $\sin x$ plus a constant this is a general solution because I can take any value of that constant and it will still satisfy this differential equation. So, any choice of this constant will still satisfy the differential equation. So, this is called a general solution on

the other hand if you have a differential equation that does not have any arbitrary constant then you call it a particular solution. So, a general solution has arbitrary constant.

Now, suppose I take the same differential equation equal to $\cos x$, but I give some boundary condition y of 0 equal to 0 suppose I say y of 0 is 0 . So, this differential equation with this boundary condition then you will say that y is equal to $\sin x$ plus c now you will say y of 0 equal to 0 ; that means, 0 equal to $\sin 0$ plus c implies c equal to 0 . So, the particular solution has the form y equal to $\sin x$. So, this is the particular solution it has no arbitrary constant. So, you can have both general and particular solutions of differential equations. So, now, what is the general strategy for solving differential equation? So, the first thing that you try to do when you get a first order differential equation is to separate variables k .

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Separation of variables

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$$\frac{dy}{dx} = 3xy + 2x$$

$$\frac{dy}{dx} = x(3y+2)$$

$$\frac{dy}{(3y+2)} = x dx$$

$$\int \frac{dy}{3y+2} = \int x dx = \frac{x^2}{2}$$

$$\frac{\log(3y+2)}{3} = \frac{x^2}{2} + C$$

$$\log(3y+2) = \frac{3x^2}{2} + C'$$

$$3y+2 = e^{\frac{3x^2}{2}} e^{C'}$$

$$3y+2 = A e^{\frac{3x^2}{2}}$$

So, for example, if you have $\frac{dy}{dx}$ is equal to $3xy$ plus, let us say $2x$ I will just say $3xy$ plus $2x$ then what you will do is you will try to write this in the following form you will write it as $\frac{dy}{dx}$ is equal to x times $3y$ plus 2 then what you will do is you will write $\frac{dy}{dx}$ divided by you will collect all the y terms on 1 side $3y$ plus 2 is equal to x $\frac{dy}{dx}$ and once you do this then you have the solution of the differential equation because you can integrate both sides independently then you integrate both sides. So, when you

integrate both sides when you integrate the left hand side integral $\frac{dy}{3y+2}$ is equal to $\log|3y+2| + C$.

So $\log|3y+2|$, if you take the derivative of \log you will get $\frac{1}{3y+2}$ and then the derivative of $3y+2$ is just 3. So, $\log|3y+2|$ divided by 3 is exactly this quantity and what about integral $x^2 dx$ this is just $\frac{x^3}{3}$. So, I can write my i. So, if I integrate both sides then I will get something like $\log|3y+2|$ divided by 3 is equal to $\frac{x^3}{3}$. Now you can always add an arbitrary constant because you take derivative of a constant you get 0. So, I can always add an arbitrary constant of integration.

So, I can rearrange this to write this as $3y+2 \log|3y+2|$ is equal to $x^3 + C$. C is some other constant C' I will just call it some other arbitrary constant C' and if you want you can even go one step further and you can write you can write $3y+2$ is equal to $e^{\frac{x^3 + C'}{3}}$ and then you have $e^{\frac{x^3 + C'}{3}}$.

So, I will just call it, I will just call it $e^{\frac{x^3 + C'}{3}}$ and $e^{\frac{x^3 + C'}{3}}$ is another arbitrary const finally, I can write the whole thing as $3y+2$ is equal to some constant $a e^{\frac{x^3 + C'}{3}}$ and if you want I can further write y equal to something, but this is how this is the general strategy of solving differential equation you try to separate variables you try to get one side having only x and one side having only y and then you integrate both sides. So, this is the basic strategy, but sometimes you cannot do this separation. So, we need other method which is what I will discuss in the next class.