Partial and (extra)ordinary differential equations and systems for chemists

Julie Rowlett

🐾

Contents

Chapter 1

Classification of ODEs and PDEs

1.1 Motivation

Why is mathematics in general and differential equations in particular important for chemistry and physics? Mathematics allows us to quantify natural phenomena and make predictions. For example, we might wish to know:

1. How much of each chemical do I need to obtain a certain chemical reaction?

2. How much of the product will I then obtain from this chemical reaction?

3. What temperature do I need for my reaction?

4. In biology and medicine: how much of a particular medication do I need for a particular patient to treat their condition?

Math offers incredible predictive power and can be used to answer questions like these. Chemical reactions generally look like

$$A + B \to C.$$
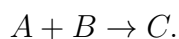
(Or do I remember this right - it has been a long time since I studied chemistry... I really liked it though!) During this process, the two compounds A and B combine to create C. While this is going on, the *amounts* of A, B, and C are changing over time. Whenever quantities are changing over time, we can describe them using differential equations! Differential equations are all about understanding quantities which change over time. If we can actually *solve* a differential equation, then we can *predict* these quantities at any point in time. Hence - the aforementioned incredible predictive power of mathematics!

1.2 Ordinary differential equations

Even though they are called ordinary, they really are anything but ordinary. Maybe we should call them extraordinary differential equations?

Definition 1.2.1 (eODE). *An "(extra)-ordinary differential equation" is an equation for an unknown function which depends on one variable.*

Inspired by crime shows, I like to call the unknown function in an eODE the "unsub." We use the variable u to represent the "unsub." Here are some examples:

1. $u'' = u$. Equivalently, we can write this ODE as $u'' - u = 0$. Note here that we don't always write the independent variable. If the independent variable is time, denoted by t, then we could write the same equation as

$$u''(t) - u(t) = 0.$$

   One reason we can omit the t (no tea no shade) is because the function u depends only on *one* variable. So this shouldn't cause any confusion.

2. Another ODE is:
$$u^2 = u.$$

   An ODE is an equation for an unknown function of one variable, so it doesn't *necessarily* contain the derivative of the unknown function.

3. Here is an ODE:
$$t^2 u''(t) + t u'(t) + u(t) = 0.$$

4. Another ODE is:
$$u'' + \lambda u = 0,$$

   where $\lambda \in \mathbb{C}$ is a constant. An example of this type is:

$$u'' + 100u = 0.$$

5. The ODE:
$$u'' = 0$$

   we solved this morning. Let's recall how we did that.

6. We also saw how to obtain all the solutions to the ODE:

$$au'' + bu' + cu = 0,$$

   Let's recall how to do this here as well.

1.2.1 Classifying eODEs

To *classify* an eODE is a way to give it a name. What's in a name? Would not a rose by any other name smell as sweet? Indeed, a rose by any other name would smell as sweet. However, if we want to search for information about roses, it really helps to know that a rose is called a rose. If we wanted to know about roses, but we didn't know what they are called, how on earth could we do a google search? I suppose you could photograph a rose with your phone and find some app which identifies flowers? To do this, you would at least need to know that a rose is a flower (i.e. you would need to know the word "flower" and what it means). Or, perhaps it would suffice to know that a rose is a plant, and then look for an app which identifies plants. In any case, you need some *key words* to be able to search for information.

It is the same idea with eODEs. I would like to teach you how to give names to the different kinds of eODEs. In this way, if you encounter them in your career as a chemist, you will be able to search for information about them. It does not help to search for information about a second order linear eODE if the equation you have is a fourth order non-linear eODE. What is true for second order linear eODEs does not apply whatsoever to fourth order non-linear eODEs! So, we need to learn how to distinguish between the different types of eODEs.

1. Look in the equation. Look for the highest derivative. This is the *degree* of the eODE.

2. Next, look in the equation and see what it is doing to u and its derivatives. In particular, the eODE is *linear* if and only if it is a linear combination of u and its derivatives. So, nothing like

$$u^2$$

   is allowed. Similarly

$$u^u$$

   is strictly forbidden. If the equation is not linear, then well, we call it *non-linear.*

1.2.2 Examples

Determine the degree of these eODEs, and also whether or not they are linear:

$$y' = 1 + y^2$$

$$y' = ay(b - y)$$

$$t x \dot{x} = 1$$

$$y' = xy$$

$$y' = 1 - y^2$$

$$x^2 y' + y = 0$$

$$y''' + 3y'' + 3y' + y = 0$$

$$y'''' + 4y''' + 6y'' + 4y' + y = 0$$

An alternative way to think about differential equations is to use the notion of *an operator.*

Definition 1.2.2. *Every eODE has a canonically associated eODE operator, L. To determine the canonically associated eODE operator, L, the eODE should be re-arranged to the form*

$$L(u) = f,$$

where f is an explicitly specified (known) function.

The idea here is that one takes u and all its derivatives, and shoves them over to the left side of the equation. The right side of the equation is a known function (which could very well be simply 0, the constant $= 0$ function). Each term on the left side of the equation can involve the independent (input) variable of the unknown function, x, as well as the unknown function u, and its derivatives. All of this collected together defines the ODE operator, L. The right side of the equation must not contain either the unknown function, u, nor any of its derivatives. We consider some of the examples above:

1. The eODE $u'' = u$ is of order two. To write the eODE $u'' = u$ using an operator, we re-write it $u'' - u = 0$. The operator is then defined to be in this case

$$L(u) = u'' - u.$$

The ODE is

$$L(u) = 0.$$

In this case, $f = 0$.

2. The eODE $u^u + u^2 = u$ is an eODE of order *zero.* This is because the unknown function (zero-th order derivative) appears in the eODE, but there are no first or higher order derivatives in the eODE. To write this eODE using an operator, we re-arrange it to

$$u^u + u^2 - u = 0, \quad L(u) = u^u + u^2 - 2.$$

3. Another eODE is: $u'' + \lambda u = 0$. For this eODE, the operator is $L(u) = u'' + \lambda u$, where λ is a constant.

4. The eODE $u' = 0$ is a first order eODE.

5. What is the order of the eODE, $u = 0$?

These examples motivate another definition.

Definition 1.2.3. *Let L be an eODE operator, with associated eODE*

$$L(u) = f(x).$$

We say that the eODE is homogeneous, *if and only if $f(x) \equiv 0$.*

Why we are bothering to introduce all of these notations and definitions? This is an intelligent thing to be asking at this point. The reason we are doing this is because the aim of this chapter is to *classify* eODEs, and later PDEs. Classifying eODEs and PDEs is a method which gives a precise, technical description of *every eODE and PDE in the universe.* There are different tools and techniques which are useful for solving different classes, or types, of eODEs and PDEs. However, the tools and techniques which can solve one type of eODE or PDE could fail miserably to solve other types of eODEs and PDEs. One would like to avoid such failures. Knowing what kind of eODE or PDE one is trying to solve, by *classifying the equation,* facilitates being able to solve it!

1.3 Classification of eODEs

Recall that a linear function, f, of several variables, x_1, x_2, ..., x_n, can always be expressed as

$$f(x_1, x_2, \ldots, x_n) = \sum_{j=1}^{n} a_j x_j, \quad a_j \in \mathbb{R} \,(\text{or } \mathbb{C}) \text{ for } j = 1, \ldots, n.$$

We shall analogously define *linear* operators.

Definition 1.3.1. *Ane ODE operator, L, is* linear *if it can be written as a linear combination of the unknown function, u, and its derivatives. A linear eODE operator, L, of order n can always be expressed as*

$$L(u) = \sum_{j=1}^{n} a_j(x) u^{(j)}.$$

Above, u denotes the unknown function, and $u^{(j)}$ denotes the jth derivative of u, where $u^{(0)} = u$. The coefficient functions $a_j(x)$ are specifically given by the eODE. A linear eODE operator L has constant coefficients *if and only if each of the functions $a_j(x)$ is a constant function.*

In the following chapter, we will see a method that will allow us to:

1. determine whether *any* homogeneous, linear eODE with constant coefficients is solvable or it is not solvable;

2. for every solvable such eODE, determine all its solutions.

These techniques are pretty powerful, and surprisingly simple once one gets accustomed to them. Before we get ahead of ourselves, let's consider some examples.

Exercise 1. *Determine in each case the eODE operator, L, and its order. Is L linear or not? Is the eODE homogeneous or not?*

1. $u' + u'' = 0$.

2. $e^u + 1 = 0$

3. $4x^2 u''(x) + 12x u'(x) + 3u(x) = 0$.

4. $2tu'4u = 3$

5. $\frac{u'(x)}{u(x)} = e^x$

6. $u'(x) = \frac{x}{u(x)}$

7. $u''(x) = 5$

8. $u'(x) = x^2$

9. $u'(x) + 5u(x) = 2$

10. $u'' = -u$

At this point, one should be able to flip open any book on eODEs and execute the following tasks:

1. identify the eODE operator, L, and its order,

2. determine whether or not L is linear,

3. determine whether or not the eODE is homogeneous.

1.4   Classification of PDEs

Partial differential equations are called so because they involve *partial* derivatives. Partial derivatives are only relevant in the context of functions of several variables. For the sake of simplicity, we will keep things real, that is in $\mathbb{R}$ and $\mathbb{R}^n$. Analysis of several complex variables is a rich and fascinating subject, but it deserves its own treatment which is beyond the scope of this mini-course.

Definition 1.4.1. *A partial differential equation (PDE) for a function of n real variables is an equation for an unknown function $u : \mathbb{R}^n \to \mathbb{R}$. The* order *of the PDE is the order of the highest partial derivative (or mixed partial derivative) which appears in the equation.*

Here are some examples:

1. For a function $u : \mathbb{R}^2 \to \mathbb{R}$, the equation, $u_{xx} + u_{yy} = 0$. What order is this equation?

10

2. For a function $u : \mathbb{R}^n \to \mathbb{R}$, the equation,

$$\sum_{j=1}^{n} u_{jj} = \lambda u, \quad \lambda \in \mathbb{R}.$$

What order is this equation?

3. For $u : \mathbb{R}^3 \to \mathbb{R}$, the equation

$$u_{xyz} - e^x u_x = \sin(yz).$$

What order is this equation?

We can also express partial differential equations using *operators,* and this will be quite useful.

Definition 1.4.2. *For a PDE of n real variables of order m, the associated PDE operator, L, is defined so that the equation is equivalent to*

$$L(u) = f,$$

where f is an explicitly specified function, with $f : \mathbb{R}^n \to \mathbb{R}$. The PDE is homogeneous if and only if $f \equiv 0$.

To familiarize oneself with the definition, recall the preceding examples of PDEs and determine the associated PDE operator, L, and specify whether or not the PDE is homogenous.

1.4.1 Classification of second order linear PDEs in two variables

As we have seen in Fourier Analysis, second order linear PDEs in two variables are in fact very important, even if they may seem simple. They are in fact, not that simple, but tractable. For problems in higher dimensions, it may often occur that the "action" is only really occurring in one space direction. Thus, for the laws of physics (and the laws which chemistry obeys as well), we only need to consider one space variable and one time variable: two variables total. Another way in which we are dealing with a three dimensional problem, but the problem can be reduced to a one (space) dimensional problem plus the time variable, is when we are able to separate the different space directions and deal with them individually.

Why is it that so many important PDEs and eODEs (like those with names) are of order two? This is due to *the laws of physics,* so many of which are written with second order PDEs and eODEs. Hence, when we want to understand the behavior of physical (and chemical) systems, we use the laws of physics to describe these systems, and many of these laws are written in the language of PDEs and eODEs. Luckily, many of these laws also happen to be *linear* PDEs. There are some important equations which are *non-linear,* but those are much more difficult to solve. However, a standard way to attack such problems is to *linearize*

them, that is to approximate the non-linear problem using a linear problem. It is therefore important to non-linear problems as well to be fluent in the methods used for solving linear PDEs.

To be able to apply the most relevant methods, it helps to be able to specify what type of equation one would like to understand. Imagine trying to search in a library or scholarly database: one needs some *terminology* in order to begin searching! We already have built up some very useful terminology for classifying equations:

1. is it an eODE or a PDE?

2. What order is the equation?

3. Is the equation linear or non-linear?

4. Is the equation homogeneous or inhomogeneous?

There are a few additional considerations and specifications for second order linear PDEs in two variables. A second order linear PDE in two independent variables, written x and y, can always be written as:

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = G, \quad A, \ldots, G \text{ are functions of } x \text{ and } y.$$

A few important examples are:

1. the heat equation, $u_t = u_{xx}$, which has $A = 1$, $E = -1$, and the other capital letters, B, C, D, F, G are all equal to zero. Note that here $y = t$ is the time variable, whereas $x \in \mathbb{R}$ or x in some bounded subset of $\mathbb{R}$ is the spatial variable.

2. The wave equation, $u_{tt} = u_{xx}$. Setting $y = t$, the time variable, what are the values of the coefficients here?

3. Laplace's equation: $u_{xx} + u_{yy} = 0$. Same question: what are the values of the coefficients in this case?

More generally, we have the following classifications:

1. Parabolic: if $B^2 - 4AC = 0$.

2. Hyperbolic: if $B^2 - 4AC > 0$.

3. Elliptic: if $B^2 - 4AC < 0$.

4. None of the above.

If at least one of the coefficients, A, B, C is non-constant, it could happen that none of the above hold. However, if these three coefficients are all constant, clearly one of the three conditions above must hold.

Exercise 2. *Classify the heat equation, wave equation, and Laplace equation.*

Exercise 3. *Classify the following equations:*

   1. $u_t = u_{xx} + 2u_x + u$

   2. $u_t = u_{xx} + e^{-t}$

   3. $u_{xx} + 3u_{xy} + u_{yy} = \sin(x)$

   4. $u_{tt} = uu_{xxxx} + e^{-t}$

Exercise 4. *Investigate solutions of the form*

$$u(x,t) = e^{ax+bt}$$

to the equation

$$u_t = u_{xx}.$$

Exercise 5. *Solve:*

$$\frac{\partial u(x,y)}{\partial x} = 0.$$

Exercise 6. *Solve:*

$$\frac{\partial^2 u(x,y)}{\partial x \partial y} = 0.$$

Compare with the eODE $u''(t) = 0$. How many solutions are there to the ODE, and what are they? How many solutions are there to the PDE (above)? Describe them.