# Partial and ordinary differential equations and systems for chemists

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# 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

$$A + B \to C.$$

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** (ODE)**.** *An "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 ODE 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:

$$t^2 u''(t) + tu'(t) + u(t) = 0.$$

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 ODEs

To *classify* an ODE 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 ODEs. I would like to teach you how to give names to the different kinds of ODEs. 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 ODE if the equation you have is a fourth order non-linear ODE. What is true for second order linear ODEs does not apply whatsoever to fourth order non-linear ODEs! So, we need to learn how to distinguish between the different types of ODEs.

**What is the order?**

1. Look in the equation. Look for the highest derivative. This is the *order* of the ODE, and is also called the *degree* of the ODE.

2. Next, look in the equation and see what it is doing to $u$ and its derivatives. In particular, the ODE 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 ODEs, and also whether or not they are linear:

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

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

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

$$y' = xy$$

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

$$x^2y' + y = 0$$
$$y''' + 3y'' + 3y' + y = 0$$
$$y'''' + 4y''' + 6y'' + 4y' + y = 0$$

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

**Definition 1.2.2.** *Every ODE has a canonically associated differential operator, $L$. To determine the canonically associated ODE operator, $L$, the ODE 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 ODE $u'' = u$ is of order two. To write the ODE $u'' = u$ 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 ODE $u^u + u^2 = u$ is an ODE of order *zero.* This is because the unknown function (zero-th order derivative) appears in the ODE, but there are no first or higher order derivatives in the ODE. To write this ODE using an operator, we re-arrange it to

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

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

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

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

These examples motivate another definition.

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

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

*We say that the ODE 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* ODEs, and later PDEs. Classifying ODEs and PDEs is a method which gives a precise, technical description of *every ODE and PDE in the universe.* There are different tools and techniques which are useful for solving different classes, or types, of ODEs and PDEs. However, the tools and techniques which can solve one type of ODE or PDE could fail miserably to solve other types of ODEs and PDEs. One would like to avoid such failures. Knowing what kind of ODE or PDE one is trying to solve, by *classifying the equation,* facilitates being able to solve it!

## 1.3 Classification of ODEs

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.** *An ODE operator, $L$, is* linear *if it can be written as a linear combination of the unknown function, $u$, and its derivatives. A linear ODE 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 $j^{th}$ derivative of $u$, where $u^{(0)} = u$. The coefficient functions $a_j(x)$ are specifically given by the ODE. A linear ODE 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 ODE with constant coefficients is solvable or it is not solvable;
2. for every solvable such ODE, 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 ODE operator, $L$, and its order. Is L linear or not? Is the ODE homogeneous or not?*

1. $u' + u'' = 0.$
2. $e^u + 1 = 0$
3. $4x^2u''(x) + 12xu'(x) + 3u(x) = 0.$
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 ODEs and execute the following tasks:

1. identify the ODE operator, $L$, and its order,
2. determine whether or not $L$ is linear,
3. determine whether or not the ODE 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.

**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?

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 $f \equiv 0$. The PDE is* linear *if and only if $L(u)$ has the form*

$$L(u) = \sum_{|\alpha| \leq m} c_\alpha(x) \partial_\alpha u.$$

*It has constant coefficients if and only if $c_\alpha(x)$ is constant for all $\alpha$. Above, $\alpha$ is a multi-index of length at most $m$, so that if $\alpha$ is a multi-index of length $k$, then $\alpha$ is of the form $j_1 \ldots j_k$, and*

$$\partial_\alpha u = \partial_{j_1} \ldots \partial_{j_k} u,$$

*where $\partial_{j_1}$ is the partial derivative in the $j_1$ coordinate direction.*

### 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 ODEs (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 ODEs. 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 ODEs. 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 ODE or a PDE?
2. What order is the equation?
3. Is the equation homogeneous or inhomogeneous?
4. Is the equation linear or non-linear?
5. If the equation is linear, the does it have constant coefficients or not?

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

# Chapter 2

# Systems of ODEs

Some Chalmers students may recall the Matlab project, Enzymkinetik, which contained the unknown concentrations of four substances each as functions of time. To determine the concentrations of these substances one must therefore solve a system of four first order ODEs. There are many other circumstances in science and engineering which may arise in which we have several functions representing quantities that depend on one another. In a chemical reaction involving 10 different molecules, the quantities of all of these different molecules depend on each other in a specific way. The way in which they depend on each other can be expressed using differential equations! Many of these systems could be *non-linear* which will create some difficulties. However, the first step to understanding non-linear ODEs (and PDEs) is actually to understand their simpler, linear versions. So, we continue to consider linear, constant coefficient homogeneous equations here.

## 2.1 Systems of ODEs in matrix-vector form

**Definition 2.1.1.** *A first-order homogeneous system of constant coefficient, linear ODEs, with $n$ unknown functions $u_1, \ldots, u_n$, which each depend on one independent variable, often denoted by $t$, is an equation*

$$U' = MU, \quad U := \begin{bmatrix} u_1 \\ u_2 \\ \cdots \\ u_n \end{bmatrix},$$

*where $M$ is an $n \times n$ matrix.*

This equation looks a lot like the single differential equation

$$f' = cf, \quad c \text{ is a constant.}$$

Solutions to that equation are $f(x) = ae^{cx}$ where $a = f(0)$. So, it makes sense to look for a vector version of such a solution for the matrix-vector equation

$$U' = MU.$$

In particular, let's first try a vector of the form

$$U = \begin{bmatrix} c_1 e^{r_1 t} \\ c_2 e^{r_2 t} \\ \vdots \\ c_n e^{r_n t} \end{bmatrix}.$$

Then

$$U' = \begin{bmatrix} r_1 & 0 & \dots & 0 \\ 0 & r_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & r_n \end{bmatrix} U.$$

Let us call the matrix

$$R = \begin{bmatrix} r_1 & 0 & \dots & 0 \\ 0 & r_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & r_n \end{bmatrix}.$$

So, the equation is satisfied if and only if

$$U' = RU = MU \iff U = R^{-1}MU.$$

The inverse matrix

$$R^{-1} = \begin{bmatrix} r_1^{-1} & 0 & \dots & 0 \\ 0 & r_2^{-2} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & r_n^{-1} \end{bmatrix}$$

OBS! The inverse matrix is usually WAY more difficult to calculate. The reason this one is so simple is because the matrix is diagonal. Now, in order to have

$$U = R^{-1}MU \implies R^{-1}M = \text{ the identity matrix,}$$

which has ones on the diagonal and zeros everywhere else. By definition of inverse matrix, then

$$M = R.$$

So, a vector of this form is only a solution when the matrix $M$ is a diagonal matrix. When $M$ is a diagonal matrix, then the system of equation looks like:

$$u_1' = r_1 u_1$$

$$u_2' = r_2 u_2$$

$$\vdots$$

$$u_n' = r_n u_n.$$

In particular, these are just $n$ equations that have nothing to do with each other. It's not super interesting, and we know how to solve these. What about when $M$ is not of this form?

For general $M$, we will look for solutions of the form

$$U = Ve^{\lambda t}, \quad V \in \mathbb{C}^n, \quad \lambda \in \mathbb{C}.$$

Then

$$U' = V\lambda e^{\lambda t} = MU \iff V\lambda e^{\lambda t} = MVe^{\lambda t}.$$

Dividing both sides of the last equality by $e^{\lambda t}$, we see that a function $U = Ve^{\lambda t}$ is a solution to the equation if and only if

$$MV = \lambda V.$$

This holds if and only if $V$ is an eigenvector for the matrix $M$, and $\lambda$ is the corresponding eigenvalue. Note that for $U$ of this type,

$$U(0) = V.$$

**Theorem 2.1.2.** *Let $M$ be an $n \times n$ matrix. Then the eigenvalues of $M$ are the roots of its characteristic polynomial*

$$p(x) = \det(M - xI),$$

*where $I$ is the $n \times n$ identity matrix. There are precisely $n$ eigenvalues, counting multiplicity, denoted by $\lambda_1, \lambda_2, \ldots \lambda_n$, with*

$$p(x) = a \prod_{j=1}^{n} (x - \lambda_j),$$

*for a constant $a \in \mathbb{C}$, with each of $\lambda_j \in \mathbb{C}$ for $j = 1, \ldots, n$. The eigenvalues which occur precisely once are* simple. *Each eigenvalue has one or more corresponding eigenvectors, so that for an eigenvalue $\lambda$, there is at least one vector $V \in \mathbb{C}^n$ with*

$$MV = \lambda V.$$

**Exercise 7.** *Show that if $M$ has real valued matrix entries and $\lambda \in \mathbb{C}$ is an eigenvalue of $M$, then $\overline{\lambda}$ is also.*

The eigenvalues of the $n \times n$ matrix, $M$, are the roots of its *characteristic polynomial,*

$$p(x) = \det(M - xI).$$

Above, $I$ is the $n \times n$ identity matrix, which has ones along the diagonal and zeros everywhere else. The polynomial $p(x)$ is a polynomial of degree $n$. By the Fundamental Theorem of Algebra, the characteristic polynomial factors over $\mathbb{C}$, so that

$$p(x) = a \prod_{j=1}^{n} (x - \lambda_j), \quad \lambda_1, \ldots, \lambda_n \in \mathbb{C}.$$

The numbers $\lambda_j$ don't need to be different, they could all be the same. For example, the matrix

$$M = I \implies p(x) = \det(I - xI) = (1-x)^n = (-1)^n \prod_{j=1}^{n} (x-1) \implies \lambda_1 = \lambda_2 = \ldots = \lambda_n = 1.$$

The number of times a specific number appears in the list $\lambda_1, \ldots, \lambda_n$ is its *algebraic multiplicity.*

Actually finding the eigenvalues of a matrix is pretty annoying, and it becomes more and more annoying the larger the matrix is. Fortunately, matrices come up all over the place; did you know that Google is fundamentally based on really large matrices? So, the good news is that one must simply stick the matrix into a computer program or a sophisticated calculator, and technology does the annoying work. The skills required by the human are thus reduced to the following tasks:

1. Do the individual equations each only have one unknown function in them? If so, then we can solve all the equations individually.

2. If not, then put the system of first order equations into matrix-vector form, defining $M$ and $U$ as above according to your equations. (If the matrix is diagonal then the individual equations only have one unknown function in each, so return to step one).

3. Ask a computer to find the eigenvectors and eigenvalues of the matrix.

4. If there are no initial conditions, then any
$$Ve^{\lambda t},$$
such that $V$ is an eigenvector with eigenvalue $\lambda$ is a solution.

5. If the initial condition, $U(0)$ is specified, then there is a solution if and only if there is an eigenvector $V$ asuch that
$$U(0) = V$$
If so, then $U(t) = Ve^{\lambda t}$ is the solution, where $\lambda$ is the eigenvalue for $V$.

A more sophisticated way to explain the last condition above is that we are checking to see if the initial data $U(0)$ is in one of the eigenspaces. For an eigenvalue $\lambda$, the eigenspace associated to $\lambda$ is the span of all the eigenvectors which have eigenvalue equal to $\lambda$.

### 2.1.1 Turning a higher order ODE into a system of first order ODEs

Another way to obtain a first-order homogeneous system of constant coefficient, linear ODEs is to start with a higher order ODE. For example, consider the equation

$$u''' + 2u'' - u' + 3u = 0.$$

**Exercise 8.** *Classify the above equation.*

This is a linear, homogeneous ODE with constant coefficients. We can use the same matrix-system technique to solve this higher order equation in the following way. Let $u_0 = u$, $u_1 = u'$, $u_2 = u''$. We can write the ODE as

$$u_0' = u_1, \quad u_1' = u_2, \quad u_2' = -2u_2 + u_1 + 3u_0.$$

Let

$$U = \begin{bmatrix} u_0 \\ u_1 \\ u_2 \end{bmatrix}.$$

The equation is now

$$U' = \begin{bmatrix} u_1 \\ u_2 \\ 3u_0 + u_1 - 2u_2 \end{bmatrix} = MU,$$

where

$$M = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 3 & 1 & -2 \end{bmatrix}.$$

To solve the system:

1. Begin by classifying the ODE. Make sure it is linear, has constant coefficients, and is homogeneous. Assume it has degree $n$.

2. Define

$$U = \begin{bmatrix} u_0 \\ u_1 \\ \dots \\ u_{n-1} \end{bmatrix}$$

with

$$u_0 = u, \quad u_1 = u', \dots, u_{n-1} = u^{(n-1)},$$

where $u$ is the unknown function we seek to satisfy the ODE.

3. Look at the ODE. Re-arrange it to look like:

$$u^{(n)} = \dots,$$

where the right side contains $u$ and its derivatives of order *less than* $n$.

4. Remember that, the way we've defined things,

$$\begin{aligned} u_0' &= u_1 \\ u_1' &= u_2 \\ u_2' &= u_3 \\ &\vdots \\ u_{(n-1)}' &= u^{(n)} = \ldots \text{ terms with } u_0,\ u_1, \text{ and up to } u_{n-1}. \end{aligned} \tag{2.1.1}$$

Collect these equations to define a matrix $M$ such that the ODE is equal to

$$U' = \begin{bmatrix} u_0' \\ u_1' \\ \cdots \\ u_{n-1}' \end{bmatrix} = MU = M \begin{bmatrix} u_0 \\ u_1 \\ \cdots \\ u_{n-1} \end{bmatrix}.$$

5. Use software to find the eigenvalues and eigenvectors of $M$.

**Exercise 9.** *Put the following systems of ODEs into matrix form:*

*1.* $u_1' = 4u_1 + 7u_2$ *und* $u_2' = -2u_1 - 5u_2$

*2.* $u_1' = 3u_2 + u_3,\ u_2' = u_1 + u_2 + u_3,\ u_3' = 0.$

*Put the following higher order ODEs into matrix form:*

*1.* $2y'' - 5y' + y = 0$

*2.* $y^{(4)} - 3y'' + y' + 8y = 0$

**Tip:** In order for a system of ODEs to be solvable, one requires the same number of *linearly independent* equations as the number of unknown functions. The reason for this is that to use a matrix and its eigenvalues, one needs the matrix to be square, that is the same number of columns as rows. There is no such thing as the eigenvalue or eigenvector of a non-square matrix. Once the system of ODEs has been put into matrix form, as

$$U' = MU,$$

then one solves for the eigenvalues of $M$ and corresponding eigenvectors.

### 2.1.2 Summary

For a system of first order, linear, homogeneous ODES (whether it came from a higher order ODE or not), write it as

$$U' = MU,$$

where $M$ is a matrix.

1. Is $M$ an $n \times n$ matrix for some $n \in \mathbb{N}$? If the answer is *yes,* then we can continue to find the solutions. If the answer is no, then we stop.

2. In case $M$ is an $n \times n$ matrix, use some technological assistance to find all its eigenvalues and corresponding eigenvectors.

3. General solutions, without any specified data, are all functions of the form

   $$U(t) = Ve^{\lambda t},$$

   such that $V$ is in the eigenspace of $\lambda$, and $\lambda$ is an eigenvalue of $M$.

4. To find a *particular solution,* we need to know the initial data,

   $$U(0).$$

   There exists a particular solution if and only if for some eigenvalue $\lambda$, $U(0)$ is contained in the eigenspace of $\lambda$. (Remember the eigenspace is the span if the eigenvectors who have eigenvalue equal to $\lambda$.)

## 2.2 The magical Laplace transform

Later in this course, we will learn about something known as the *Laplace transform.* It is defined for functions which do not grow super-exponentially.

**Definition 2.2.1.** *Assume that*

$$f(t) = 0 \quad \forall t < 0, \tag{2.2.1}$$

*and that there exists $a, C > 0$ such that*

$$|f(t)| \leq Ce^{at} \quad \forall t \geq 0. \tag{2.2.2}$$

*Then for we define for $z \in \mathbb{C}$ with $\Re(z) > a$ the Laplace transform of $f$ at the point $z$ to be*

$$\mathfrak{L}f(z) = \int_0^\infty f(t)e^{-zt}dt.$$

**Exercise 1.** *Show that if $f$ is continuous and piecewise $\mathcal{C}^1$ on $[0, \infty)$, and $f'$ satisfies* (2.2.2) *and* (2.2.1)*, then*

$$\mathfrak{L}(f')(z) = z\mathfrak{L}f(z) - f(0).$$

*(Hint: integrate by parts!)*

The Laplace transform can be used to solve any linear, constant coefficient ODE, whether it is homogeneous or not! This is super amazing. Time permitting, we will learn how to do this here.

**Proposition 2.2.2.** *Assume that everything is defined, then*

$$\mathfrak{L}(f^{(k)})(z) = z^k \mathfrak{L}f(z) - \sum_{j=1}^{k} f^{(k-j)}(0) z^{j-1}.$$

**Proof:** Well clearly we should do a proof by induction! Check the base case first:

$$\mathfrak{L}(f')(z) = z\mathfrak{L}f(z) - f(0).$$

Here $k = 1$ and the sum has only one term with $j = k = 1$. It works. Now we assume the above formula holds and we show it for $k + 1$. We compute

$$\mathfrak{L}(f^{(k+1)})(z) = \mathfrak{L}((f^{(k)})')(z) = z\mathfrak{L}(f^{(k)})(z) - f^{(k)}(0).$$

By induction this is

$$z\left(z^k \mathfrak{L}f(z) - \sum_{j=1}^{k} f^{(k-j)}(0) z^{j-1}\right) - f^{(k)}(0).$$

This is

$$z^{k+1}\mathfrak{L}f(z) - \sum_{j=1}^{k} f^{(k-j)}(0) z^{j} - f^{(k)}(0).$$

Let us change our sum: let $j + 1 = l$. Then our sum is

$$\sum_{l=2}^{k+1} f^{k-(l-1)}(0) z^{l-1} = \sum_{l=2}^{k+1} f^{(k+1-l)}(0) z^{l-1}.$$

Observe that

$$f^{(k)}(0) = f^{k+1-1}(0) z^{1-1}.$$

Hence

$$-\sum_{j=1}^{k} f^{(k-j)}(0) z^{j} - f^{(k)}(0) = -\sum_{l=1}^{k+1} f^{(k+1-l)}(0) z^{l-1}.$$

So, we have computed

$$\mathfrak{L}(f^{(k+1)})(z) = z^{k+1}\mathfrak{L}f(z) - \sum_{l=1}^{k+1} f^{(k+1-l)}(0) z^{l-1}.$$

That is the formula for $k + 1$, which is what we needed to obtain.

# Chapter 3

# Techniques for solving ODEs

To get warmed up, we recall some famous chemical examples, the first of which Chalmers students will recognize from the Matlab project, Enzymkinetik from the first-year course, Kemi.

## 3.1 Three chemical examples

The concentrations of reactants and products in a chemical reaction vary with time. The way in which these concentrations vary is known as *chemical kinetics* and is governed by rate laws. These rate laws relate the time derivatives of the concentrations to the concentration of the participating molecules at any given time. The simplest description of how an enzyme, $E$, catalyzes the conversion of the substrate, $S$ to the product, $P$ is given by the scheme

$$E + S \leftrightarrow ES \to P + E.$$

Above, $ES$ is an intermediate complex between $S$ and $E$. The rate constants are denoted by $c_1$ for the first forward reaction, $c_2$ for the corresponding backward reaction, and $c_3$ for the second forward reaction. Let the concentrations at time equal to $t$ be given by the four functions

$$[E](t) = u(t), \quad [S](t) = v(t), \quad [ES](t) = y(t), \text{ and } [P](t) = z(t).$$

**Exercise 10.** *Formulate the four differential equations for the situation described above for the four unknown functions $u$, $v$, $y$, and $z$. Classify each of the ODEs.*

For two chemicals, $u$ and $v$, we use $u(t)$ and $v(t)$ to denote the concentration of $u$ and $v$, respectively, at time $t$ after the reaction has begun. The general rate laws are

$$u'(t) = c_1 u(t)^a v(t)^b, \quad v'(t) = c_2 u(t)^a v(t)^b.$$

This is known as the law of mass action, with rate constants $c_1$ and $c_2$. The constants $a$ and $b$ are the reaction orders with respect to $u$ and $v$, respectively.

**Exercise 11.** *Classify the law of mass action ODE above. Note that there are a few different cases depending on the values of $a$ and $b$.*

The Robinson annulation is also a famous system of ordinary differential equations from organic chemistry for ring formation. In 1935, Robert Robinson used this method to create a six membered ring by forming three new carbon-carbon bonds. There are three chemical substances whose amounts at time $t$ are respectively

$$u_1(t), \quad u_2(t), \quad u_3(t).$$

Due to the chemical process, the abundances of these satisfy

$$u_1'(t) = -0.04u_1 + 10000u_2u_3,$$

$$u_2'(t) = 0.04u_1 - 10000u_2u_3 - 30000000u_2^2,$$

$$u_3'(t) = 30000000u_2^2.$$

**Exercise 12.** *Classify each of the ODEs in the Robinson annulation.*

The preceding two equations are often not possible to solve analytically, that is by hand. In fact, there are many more equations which we *cannot* solve analytically as compared to those which we can solve analytically. There are numerous numerical methods to determine approximate solutions to ODEs and PDEs, but the first step is always to *classify* the equation. By classifying the equation, you can look up information about that type of equation and see what resources are available to deal with it.

We'll conclude the last chapter of this note with a few more methods which one *can* use to solve first and second order ODEs. Many of the laws of physics require only first order derivatives, and can be expressed using first order ODEs. There are also many laws of physics and chemistry which involve second order derivatives and can therefore be expressed using second order ODEs. So, although these may seem quite specific, they are nonetheless physically and chemically relevant. The goal of Fourier analysis is to build up a toolbox for solving the ODEs and PDEs of physics, nature, and engineering. There are a few more techniques which could be useful to have in one's toolbox.

## 3.2 Methods for solving first order ODEs

We begin with first order ODEs. They may seem like the simplest case, but you'll see they can pack a serious surprise blow.

### 3.2.1 First order linear constant and non-constant coefficients: the M$\mu$thod

Can the equation be massaged into the form:

$$u'(t) + p(t)u(t) = g(t)?$$

Compute in this case:

$$\mu(t) := \exp\left(\int p(t)dt\right).$$

Don't worry about the constant of integration, we don't need it here. Next compute

$$\int \mu g = \int \mu(t)g(t)dt + C.$$

Don't forget the constant here! That's why we use a capital $C$. The solution is:

$$u(t) = \frac{\int(\mu g)(t)}{\mu(t)} = \frac{\int \mu(t)g(t)dt + C}{\mu(t)}.$$

To illustrate the method, we'll do some examples.

1. $tu' + 2u = t^2 - t + 1$, with $u(1) = 0$.

2. $tu' - 2t = t\sin(2t) - t^2 + 5t^4$, with $u(\pi) = \pi$.

3. $2u' - u = 4\sin(3t)$, $u(0) = u_0$.

We consider the first equation. It is not in the right form, so we need to modify if to get it in the desired form. So, we re-write it as:

$$u' + 2u/t = t - 1 + 1/t.$$

So we see that the coefficient of $u$ is

$$p(t) = 2/t.$$

This function is perfectly fine as long as $t \neq 0$. Now, our

$$\mu(t) = \exp(\int p(t)dt) = e^{2\ln(t)} = t^2.$$

Now, let's determine what $g$ is:

$$g(t) = t - 1 + 1/t.$$

We therefore compute

$$\int \mu(t)g(t)dt = \int t^2(t - 1 + 1/t)dt = t^4/4 - t^3/3 + t^2/2 + c.$$

The solution is then of the general form:

$$u(t) = \frac{t^4/4 - t^3/3 + t^2/2 + c}{t^2} = t^2/4 - t/3 + 1/2 + \frac{c}{t^2}.$$

Since $u(1) = 0$, we compute

$$1/4 - 1/3 + 1/2 + c = 0 \implies c = -5/12,$$

$$u(t) = t^2/4 - t/3 + 1/2 - \frac{5}{12t^2}$$

Now, we can check that our solution really is a solution by putting it into the ODE:

$$u'(t) = t/2 - 1/3 + 5/(6t^3).$$

$$u' + 2u/t = t/2 - 1/3 + 5/(6t^3) + t/2 - 2/3 + 1/t - \frac{5}{6t^3}$$
$$= t - 1 + 1/t.$$

To be totally honest, the first time I solved this equation, I made an error. I only found the error by plugging the solution back into the equation. So, especially if you're doing something important, it can be a good idea to plug your solution back into the ODE.

Now let's do the second equation. First, we need to re-arrange it to get it into the model form:

$$tu' = t\sin(2t) - t^2 + 5t^4 + 2 \implies u' = \sin(2t) - t + 5t^3 + 2/t.$$

Here, the function

$$p(t) = 0.$$

Not to worry, because we compute:

$$\mu(t) = e^{\int p(t)dt}) = e^0 = 1.$$

On the right side we have

$$g(t) = \sin(2t) - t + 5t^3 + 2/t.$$

We therefore compute

$$\int \mu(t)g(t)dt = \int \sin(2t) - t + 5t^3 + 2/t + c$$
$$= -\cos(2t)/2 - t^2/2 + 5t^4/4 + 2\ln(t) + c.$$

Our solution

$$u(t) = -\cos(2t)/2 - t^2/2 + 5t^4/4 + 2\ln(t) + c.$$

To determine the constant, we use the information

$$u(\pi) = \pi,$$

so

$$-\cos(2\pi) - \pi^2/2 + 5\pi^4/4 + 2\ln(\pi) + c = \pi,$$
$$\iff c = \pi + 1 + \pi^2/2 - 5\pi^4/4 - 2\ln(\pi).$$

Now, let's make sure our solution satisfies the equation:

$$u' = \sin(2t) - t + 5t^3 + 2/t.$$

**Exercise 13.** *Use the Mμthod to solve the third equation above, namely:*

$$2u' - u = 4\sin(3t), \quad u(0) = u_0.$$

### 3.2.2 Separable

If your equation is not linear, you might be so lucky that you can re-arrange it like this:

$$\Phi(u)u'(t) = g(t).$$

Such an equation is called separable. The left side is some mish mash involving $u$, expressed as $\Phi(u)$, where $\Phi$ is a function of one variable, and the right side is an explicit function of $t$ that comes from the ODE. Let us write it in this way:

$$\Phi(u)\frac{du}{dt} = g(t).$$

Then, we will write something which is not really good notation, but it is just a means to an end.[1] So, we write

$$\Phi(u)du = g(t)dt.$$

Next, we integrate both sides, that is we find a function $F(u)$ such that

$$F'(u) = \Phi(u),$$

and a function $G(t)$ whose derivative

$$G'(t) = g(t).$$

Our equation is then

$$F(u) = G(t) + C.$$

Here are some examples.

1. $\dot{u} = 6u^2 t$. We can re-write this as:

   $$\frac{\dot{u}}{u^2} = 6t.$$

   So, we put

   $$\frac{du}{u^2} = 6tdt \implies \int \frac{1}{u^2}du = \int 6tdt.$$

   We know how to compute these integrals. We get:

   $$-\frac{1}{u} = 3t^2 + C.$$

   In this case, we can actually solve for $u$,

   $$u = -\frac{1}{3t^2 + C}.$$

   If we have for instance some initial data, like the value of $u(0)$ then we can solve for $C$ and obtain

   $$C = -\frac{1}{u(0)}.$$

[1] La fin justifie les moyens, is a song by French rapper M.C. Solaar, which is really good. The title means "the end justifies the means."

2. $\sin(u)\dot{u} = 4t^2$. We shall do the same rather dirty-math means to an end:

$$\sin(u)du = 4t^2dt \implies \int \sin(u)du = \int 4t^2dt.$$

We can compute these integrals:

$$-\cos(u) = \frac{4t^3}{3} + C.$$

Again we are in luck, because we can solve for $u$:

$$u = \arccos\left(-\frac{4t^3}{3} - C\right).$$

If we know some initial data, like $u(0) = 1$, then we know that

$$\arccos(-C) = 1 \implies C = 0.$$

Hence

$$u = \arccos\left(-\frac{4t^3}{3}\right).$$

### 3.2.3 Exact

Can you express your equation this way,

$$\Psi_t(u,t) + \Psi_u(u,t)u'(t) = 0?$$

Above, the function $\Psi : \mathbb{R}^2 \to \mathbb{R}$ is a function of two variables. If you can express your function this way, then by the chain rule, $\Psi(u(t),t)$ is constant. Thus, there is a $c \in \mathbb{R}$ such that

$$\Psi(u(t),t) = c.$$

This type of equation is known as exact, and again, it only gives an *implicit* (not explicit) solution for $u$.

Let's look at some examples.

1. $2tu^2 + 4 = 2(3 - t^2u)\dot{u}$. We re-arrange the equation to

$$2tu^2 + 4 + 2(t^2u - 3)\dot{u} = 0.$$

Next, we have two parts, and we want to determine whether we can find $\Psi$ with

$$\Psi_t = 2tu^2 + 4, \quad \Psi_u = 2(t^2u - 3).$$

So, let's begin with the first part. We integrate with respect to $t$:

$$\Psi(u,t) = t^2u^2 + 4t + f(u).$$

Above, the $f(u)$ term does not have any $t$. (No tea no shade). Next, we take our candidate and differentiate with respect to $u$, getting

$$2t^2u + f'(u).$$

We want this to equal the second part:

$$2t^2u + f'(u) = 2(t^2u - 3).$$

For this to be true, we see that we need

$$f'(u) = -6 \implies f(u) = -6u.$$

Hence, our

$$\Psi(u,t) = t^2u^2 + 4t - 6u.$$

This is equal to a constant,

$$t^2u^2 + 4t - 6u = c.$$

If we know for example $u(0) = 0$, then we can compute that $c = 0$. Hence, we have the equation

$$t^2u^2 - 6u + 4t = 0.$$

We are super lucky, because this is a quadratic expression for $u$. The solutions are

$$u = \frac{6}{2t^2} \pm \frac{\sqrt{36 - 16t^3}}{2t^2}.$$

2. $3y^3e^{3xy} - 1 + (2ye^{3xy} + 3xy^2e^{3xy})y' = 0$. Just so that you aren't surprised, we are now using $y = y(x)$ for our unknown function (unsub). We are now looking for a function $\Psi(x,y)$ such that

$$\Psi_x = 3y^3e^{3xy} - 1, \quad \Psi_y = (2ye^{3xy} + 3xy^2e^{3xy}).$$

We take the first part and integrate with respect to $x$, getting our candidate

$$\Psi(x,y) = y^2e^{3xy} - x + f(y).$$

Now, we differentiate with respect to $y$,

$$\Psi_y = 2ye^{3xy} + 3xy^2e^{3xy} + f'(y).$$

We need this to be the second part,

$$2ye^{3xy} + 3xy^2e^{3xy} + f'(y) = 2ye^{3xy} + 3xy^2e^{3xy} \implies f'(y) = 0 \implies f(y) = c \in \mathbb{R}.$$

Hence

$$\Psi(x,y) = y^2e^{3xy} - x + c.$$

Since we know that $\Psi$ is equal to the constant, we can just re-name our constant and consolidate it on the right side,

$$\Psi(x,y) = y^2e^{3xy} - x = c.$$

This time, we can't get $y$ by itself. That's okay though. We still have an *implicit* solution.

### 3.2.4 Bernoulli

Is your ODE of the form

$$u' + p(t)u = q(t)u^n, \quad n \neq 0, 1?$$

If so, let

$$v(t) := \frac{u^{1-n}}{1-n}.$$

Then the ODE is

$$v' + \widetilde{p(t)}v(t) = q(t), \quad \widetilde{p(t)} = (1-n)p(t).$$

This is now a linear first order ODE which can be solved by the M$\mu$thod.

### 3.2.5 Substitution

Is your ODE of the form

$$u' = f(u, t)?$$

Is there a function

$$v = v(u, t)$$

such that you can compare $v'$ and $u'$? In particular, is there a simple relationship between $u'$ and $v'$? The goal here is to re-write the equation in terms of $v$, so that you can use one of the preceding methods. This method can be rather subtle and tricky.

### 3.2.6 Exercises

1. $y' = \frac{3x^2+4x-4}{2y-4}$, $y(1) = 3$.
2. $y' = \frac{xy^3}{\sqrt{1+x^2}}$, $y(0) = -1$.
3. $y' = e^{-y}(2x-4)$, $y(5) = 0$.
4. $\frac{dr}{d\theta} = \frac{r^2}{\theta}$, $r(1) = 2$.
5. $\frac{dy}{dt} = e^{y-t}\sec(y)(1+t^2)$, $y(0) = 0$.
6. $2xy - 9x^2 + (2y + x^2 + 1)y' = 0$.
7. $2xy^2 + 4 = 2(3 - x^2y)y'$, $y(-1) = 8$.
8. $\frac{2ty}{t^2+1} - 2t - (2 - \ln(t^2+1))y' = 0$.
9. $y' + \frac{4}{x}y = x^3y^2$, $y(2) = -1$.
10. $y' = 5y + e^{-2x}y^{-2}$, $y(0) = 2$.
11. $6y' - 2y = xy^4$, $y(0) = -2$.

12. $y' + \frac{y}{x} - \sqrt{y} = 0$, $y(1) = 0$.
13. $xyy' + 4x^2 + y^2 = 0$, $y(2) = -7$.
14. $xy' = y(\ln(x) - \ln(y))$, $y(1) = 4$.
15. $y' - (4x - y + 1)^2 = 0$, $y(0) = 2$.
16. $y' = e^{9y-x}$, $y(0) = 0$.

## 3.3 Second order ODEs

Do you have an ODE of the form

$$ay'' + by' + cy = 0?$$

Let

$$y(x) = e^{rx}.$$

This leads to the quadratic equation

$$ar^2 + br + c = 0.$$

The solutions are

$$r = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$

There are a few cases to consider

1. $b^2 > 4ac$. Then the two linearly independent solutions are

   $$y_1 = e^{r_+x}, \quad y_2 = e^{r_-x},$$

   with

   $$r_\pm = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$

   The general solutions are

   $$c_1y_1 + c_2y_2, \quad c_1, c_2 \in \mathbb{R}.$$

2. $b^2 = 4ac$. The first solution is

   $$y = e^{rx}, \quad r = \frac{-b}{2a}.$$

   The second independent solution is

   $$z = xe^{rx},$$

   and therefore solutions in general are given by:

   $$c_1e^{rx} + c_2xe^{rx}.$$

3. $b^2 < 4ac$. In this case our solutions are complex

$$y_\pm = e^{r_\pm x} : \mathbb{R} \to \mathbb{C}.$$

The real and imaginary parts also satisfy the equation, and thus the solutions are

$$e^{-bx/a}\left(c_1 \sin\left(\frac{\sqrt{4ac-b^2}x}{2a}\right) + c_2 \cos\left(\frac{\sqrt{4ac-b^2}x}{2a}\right)\right)$$

**Exercise 14.** *Solve:*

1. $y'' - 6y' + 8y = 0$.
2. $y'' + 8y' + 41y = 0$.
3. $y'' - 2y' + y = 0$.
4. $4y'' + y = 0$.
5. $4y'' + y' = 0$.
6. $y'' + 12y' + 36y = 0, y(1) = 0, y'(1) = 1$.
7. $y'' - 2y' + 5y = 0, y(\pi) = 0, y'(\pi) = 2$.
8. $2y'' + 5y' - 3y = 0,\ y(0) = 1,\ y'(0) = 4$.
9. $y'' + 3y = 0,\ y(0) = 1,\ y'(0) = 3$.
10. $y'' + 100y = 0,\ y(0) = 2,\ y(\pi) = 5$.
11. *Let* $L \in \mathbb{R}$ *mit* $L \neq 0$. *Show that the only solution to*

$$y'' + \lambda y = 0, \quad y(0) = 0, y(L) = 0$$

*is the trivial solution* $y \equiv 0$ *for* $\lambda \leq 0$. *For the case* $\lambda > 0$, *find* $\lambda$ *such that the problem has a non-trivial solution and determine such solution(s).*

12. *Let* $a, b, c > 0$ *and* $y(x)$ *be a solution to*

$$ay'' + by' + cy = 0.$$

*Show that* $\lim_{x\to\infty} y(x) = 0$.

### 3.3.1 The Wronskian

Consider an ODE,

$$p(t)y'' + q(t)y' + r(t)y = 0,$$

and let $y_1$ and $y_2$ be solutions. It may be useful to know (but we do not need to prove it here) the following facts.

**Theorem 3.3.1.** *Let $y_1$ and $y_2$ be two solutions to the ODE*

$$p(t)y'' + q(t)y' + r(t)y = 0.$$

*The Wronskian of $y_1$ and $y_2$ is defined to be*

$$W(y_1, y_2)(t) = y_1(t)y_2'(t) - y_2(t)y_1'(t).$$

*If there is $t_0$ such that $W(y_1, y_w)(t_0) \neq 0$, then $y_1$ and $y_2$ are a basis for all solutions of the ODE. If $y_1$ and $y_2$ are linearly dependent, then $W(y_1, y_2) \equiv 0$.*

**Theorem 3.3.2.** *Assume that $y_1$ und $y_2$ are a basis of solutions to the ODE*

$$L(y) = y'' + q(t)y' + r(t)y = 0.$$

*Then a solution to the ODE*

$$L(y) = g(t)$$

*is given by*

$$Y(t) = -y_1 \int \frac{y_2 g(t)}{W(y_1, y_2)} dt + y_2 \int \frac{y_1 g(t)}{W(y_1, y_2)} dt.$$

**Exercise 15.** *Solve the following equations:*

$$2y'' + 18y = 6\tan(3t)$$

$$y'' - 2y' + y = \frac{e^t}{t^2 + 1}$$

## 3.4 The Laplace transform solves all linear constant coefficient ODEs

A linear, constant coefficient ODE of order $n$ looks like:

$$\sum_{k=0}^{n} c_k u^{(k)}(t) = f(t).$$

In order for the solution to be unique, there must be specified initial conditions on $u$, that is these must be specified

$$u(0), u'(0), \ldots u^{(n-1)}(0).$$

To solve the ODE, we hit both sides of the ODE with $\mathfrak{L}$:

$$\sum_{k=0}^{n} c_k \mathfrak{L}(u^{(k)})(z) = \widetilde{f}(z).$$

Let's write out the left side using the proposition we proved last time. First we have

$$c_0 \widetilde{u}(z).$$

Then we have

$$c_1 \left( z\widetilde{u}(z) - u(0) \right).$$

In general we have

$$c_k \left( z^k \widetilde{u}(z) - \sum_{j=1}^{k} u^{(k-j)}(0) z^{j-1} \right).$$

So, if we collect all the terms with $\widetilde{u}(z)$, we get

$$(c_0 + c_1 z + c_2 z^2 + \ldots + c_n z^n)\widetilde{u}(z) = P(z)\widetilde{u}(z),$$

$$P(z) = \sum_{k=0}^{n} c_k z^k.$$

Now let's collect all the rest:

$$-\sum_{k=1}^{n} c_k \sum_{j=1}^{k} u^{(k-j)}(0) z^{j-1} = Q(z).$$

This is just a polynomial also. So our ODE has been LAPLACE-TRANSFORMED into

$$P(z)\widetilde{u}(z) + Q(z) = \widetilde{f}(z).$$

We can solve this for $\widetilde{u}(z)$:

$$\widetilde{u}(z) = \frac{\widetilde{f}(z) - Q(z)}{P(z)}.$$

Hence to get our solution $u(t)$ we just need to invert the Laplace transform of the right side, that is our solution will be

$$u(t) = \mathfrak{L}^{-1} \left( \frac{\widetilde{f}(z) - Q(z)}{P(z)} \right).$$

# Chapter 4

# Projects

Students may work in groups of up to four people. Every group shall complete the first, warm-up project, Project 0. Then, each group shall choose one of Projects 1, 2, 3, 4, 5, 6, or X to complete in order to receive credit for this course.

## 4.1 Project 0: Create your own flow chart

The purpose of this project is to create a flow chart showing how to deal with ODEs and PDEs. Begin by classifying as an ODE or a PDE. Next, classify the ODE or PDE. If there are methods contained either in this compendium or in the Fourier Analysis course which can be used to solve the equation, the flow chart should lead to the appropriate method. If, however, we have not seen any way to analytically solve the equation, the flow chart should lead to "solve numerically." You may use any help material, the flow chart can be drawn by hand or created using software, and you are free to discuss this with anyone!

## 4.2 Project 1: Canonical forms for second order linear PDEs in two variables

The goal of this project is to play with changing coordinates in order to make PDEs look different. This may seem tedious and silly, but in fact, changing coordinates can be one of the most fruitful things one can do with a PDE! A simple change of coordinates could turn something which seemed unsolvable analytically into an equation which is a peach to solve! So, to develop this skill, you will practice transforming hyperbolic and parabolic PDEs into canonical forms.

### 4.2.1 Hyperbolic equation

Starting from the general PDE

$$au_{xx} + bu_{xy} + cu_{yy} + du_x + eu_y + fu = g,$$

we assume now that $b^2 - 4ac > 0$. The goal is to introduce new coordinates,

$$\xi = \xi(x, y), \quad \eta = \eta(x, y),$$

so that the PDE contains only one second derivative, $u_{\xi\eta}$.

**Exercise 16.** *Compute the partial derivatives $u_x$, $u_y$, $u_{xx}$, $u_{xy}$, and $u_{yy}$ in the new coordinates.*

**Exercise 17.** *Substitute the partial derivatives into the equation to create an equation*

$$\alpha u_{\xi\xi} + \beta u_{\xi\eta} + \gamma u_{\eta\eta} + \delta u_\xi + \nu u_\eta + \phi u = \Gamma.$$

*Express $\alpha$, $\beta$, and all the way up to $\Gamma$ in terms of $a, b, c, d, e, f, g$ together with the partial derivatives of the coordinates $\eta$ and $\xi$.*

**Exercise 18.** *Set the coefficients $\alpha$ and $\gamma$ equal to zero. Use this to obtain two quadratic equations for the variables*

$$\frac{\xi_x}{\xi_y} \text{ and } \frac{\eta_x}{\eta_y}.$$

*Determine the roots of each of these quadratic equations. Let $A$ be a root of the equation for $\xi$, and $B$ be a root of the equation for $\eta$. Show that*

$$\xi = y + Ax, \quad \eta = y + Bx$$

*will satisfy the equation.*

**Exercise 19.** *Write up the PDE in terms of the coordinates $\xi$ and $\eta$, and verify that indeed it only contains one second derivative, $u_{\xi\eta}$.*

**Exercise 20.** *The hyperbolic equation has two canonical forms. The second canonical form comes from introducing new coordinates*

$$w = \xi + \eta, \quad v = \xi - \eta.$$

*Determine the PDE in terms of these new coordinates.*

### 4.2.2 Parabolic equation

Starting from the general PDE

$$au_{xx} + bu_{xy} + cu_{yy} + du_x + eu_y + fu = g,$$

we assume now that $b^2 - 4ac = 0$. The goal here is to introduce coordinates $\xi$ and $\eta$, so that the equation takes the form

$$u_{\eta\eta} = \Phi(\xi, \eta, u, u_\xi, u_\eta).$$

**Exercise 21.** *Compute the Greek equation*

$$\alpha u_{\xi\xi} + \beta u_{\xi\eta} + \gamma u_{\eta\eta} + \delta u_\xi + \nu u_\eta + \phi u = \Gamma.$$

*Express $\alpha$, $\beta$, and all the way up to $\Gamma$ in terms of $a, b, c, d, e, f, g$ together with the partial derivatives of the coordinates $\eta$ and $\xi$.*

**Exercise 22.** *The goal now is to set $\beta$ and either $\alpha$ or $\gamma$ equal to zero and solve for $\eta$ and $\xi$. Do this and determine an equation for either $\xi_x/\xi_y$ or $\eta_x/\eta_y$. Find a solution, and pick the second coordinate to be linearly independent.*

## 4.3 Project 4: Fourier analysis of the hydrogen atom

The goal of this project is for you to work out, in full detail, the outline in Folland's book concerning the Fourier analysis of the hydrogen atom. This is based on Folland p. 194-195, and a reference there is Landau-Lifschitz, *Quantum Mechanics (non-relativistic theory).*

In the hydrogen atom, there is an electron and a proton. The proton is about 2,000 times more massive than the electron, so it makes sense to consider the proton as immobile, from the electron's point of view. The electron is therefore moving in an electrostatic force field with potential $-\epsilon^2/r$, where $\epsilon$ is the charge of the proton, and $r$ is the distance from the origin. We assume that the proton is located at the origin.

According to quantum mechanics, when the electron is in a stationary state at energy level $E$, its wave function $u$ is in $L^2(\mathbb{R}^3)$ and satisfies the equation

$$\frac{\hbar^2}{2m}\Delta u + \frac{\epsilon^2}{r}u + Eu = 0. \tag{4.3.1}$$

Above, $\hbar$ is Planck's constant, and $m$ is the mass of the electron, the Laplace operator $\Delta$ is in $\mathbb{R}^3$ equal to

$$\Delta = \partial_x^2 + \partial_y^2 + \partial_z^2.$$

Due to the fact that there is an $r$ in the equation, it is natural to introduce spherical coordinates.

**Exercise 23.** *Let*

$$x = r\cos\theta\sin\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\phi.$$

*Show that*

$$\Delta f = f_{rr} + \frac{2}{r}f_r + \frac{1}{r^2\sin\phi}(f_\phi \sin\phi)_\phi + \frac{1}{r^2\sin^2\phi}f_{\theta\theta}.$$

**Exercise 24.** *For a function of the form $R(r)\Theta(\theta)\Phi(\phi)$, compute*

$$\Delta(R(r)\Theta(\theta)\Phi(\phi).$$

Now, the equation (4.3.1) looks a bit more complicated than necessary. We can change the units of mass, so that we can assume $\hbar = m = \epsilon = 1$. Then, our equation becomes

$$\frac{1}{2}\Delta u + \frac{u}{r} + Eu = 0 \iff \Delta u + 2\frac{u}{r} + 2Eu = 0. \tag{4.3.2}$$

Assume our function $u = R(r)\Theta(\theta)\Phi(\phi)$.

**Exercise 25.** *Using separation of variables, show that (up to a constant multiple) the $\Theta$ part of the function must be equal to*

$$\Theta(\theta) = e^{im\theta},$$

*and that*

$$\Phi(\phi) = P_n^{|m|}(\cos\phi),$$

*where $n \geq |m|$. Above, $P_n^m$ is the* associated Legendre function,

$$P_n^m(s) = \frac{(1-s^2)^{m/2}}{2^n n!}\frac{d^{n+m}}{ds^{n+m}}(s^2-1)^n.$$

*Show that $P_n^m$ is the solution of the problem for the function $y = y(s)$ of one variable,*

$$[(1-s^2)y'] + \frac{m^2 y}{1-s^2} + n(n+1)y = 0, \quad y(-1) = y(1) = 0.$$

*Hint: see §6.3 of Folland.*

Next, we're going to consider the radial part.

**Exercise 26.** *Show that $R$ must satisfy*

$$r^2 R'' + 2rR' + [2Er^2 + 2r - n(n+1)]R = 0.$$

Let's think for a moment about the energy, $E$. A proton is positively charged. So, if the electron is also positively charged, the two of them repel each other, and the electron runs away. This does not create a hydrogen atom. So, we're interested in negative energy, $E < 0$, because this can create a bond with the proton, so that the electron stays trapped. That's what's happening in a hydrogen atom. Following Folland, we introduce some notations, because it will actually make the calculations simpler. From now on, we assume

$$E < 0.$$

Let

$$\nu = (-2E)^{-1/2}, \quad s = 2\nu^{-1}r, \quad R(r) = S(2\nu^{-1}) = S(s).$$

**Exercise 27.** *Show that the equation becomes*

$$s^2 S'' + 2sS' + [\nu s - \frac{1}{4}s^2 - n(n+1)]S = 0.$$

*Next, let*

$$S = s^n e^{-s/2} \Sigma.$$

*Show that the equation now becomes*

$$s\Sigma'' + (2n + 2 - s)\Sigma' + (\nu - n - 1)\Sigma = 0.$$

*Verify that this is the Laguerre equation,*

$$xy'' + (\alpha + 1 - x)y' + ny,$$

*with* $\alpha = 2n + 1$ *and* $n$ *replaced by* $\nu - n - 1$.

The only solutions of the Laguerre equation which will yield a function $u = R\Theta\Phi \in L^2(\mathbb{R}^3)$ are the Laguerre polynomials. You may trust this fact or dig up further justification if you are sceptical. It all comes down to completeness of the ONB of $L^2$ formed by these polynomials. That is proven by showing that any $L^2$ function can be approximated, to arbitrary precision, by these, and also by showing that these are a complete orthogonal set in $L^2$.

So we now know that $\nu \geq n + 1$ and $\nu \in \mathbb{Z}$.

**Exercise 28.** *Unravel all the substitutions to show that the solution*

$$R_{n\nu}(r) = (2\nu^{-1}r)^n e^{-r/\nu} L^{2n+1}_{\nu-n-1}(2\nu^{-1}r),$$

*and*

$$u_{mn\nu} = R_{n\nu}(r) e^{im\theta} P_n^{|m|}(\cos(\phi),$$

*with*

$$E_{mn\nu} = -\frac{1}{2}\nu^{-2}.$$

What is important to notice here is that $\nu$ is an *integer.* This means that when $\nu$ changes, the energy $E_{mn\nu}$ *jumps.* This is because any two different integers are at least one apart. Therefore, the energy can only come at the levels

$$E_{mn\nu} = -\frac{1}{2}\nu^{-2}, \quad \nu \in \mathbb{Z}, \quad \nu \geq n + 1.$$

It is rather fascinating to know that experimental physicists already knew this fact about the energy levels, before the mathematics had been done!

Another important observation is that $E_{mn\nu}$ depends only on $\nu$, as long as $\nu \geq n + 1$. So, there are a lot of different functions $u_{mn\nu}$ for each $E_{mn\nu}$. What happens to the energy as $\nu \to \infty$?

## 4.4 Project 5: Distribution Theory

In this project you will learn about the mysterious and magical *distributions*, or, as they are sometimes called, *generalized functions.* You may have already heard about the so-called "delta function." It's not really a function. It's a distribution. Now, distributions are not as mysterious and weird as the mystique in which they are often shrouded.

In order to define them in a precise way, we require a few definitions.

**Definition 4.4.1.** *An* open set $S \subset \mathbb{R}^n$ *is either the empty set, or it satisfies*

$$\forall x \in S, \quad \exists r > 0 \text{ such that } B_r(x) \subset S.$$

*Above, $B_r(x)$ means the ball centered at $x$ with radius $r$, that is the set*

$$B_r(x) = \{y \in \mathbb{R}^n \mid |x - y| < r\}$$

*. So, in words, the ball centered at $x$ with radius $r$ is the set of points $y \in \mathbb{R}^n$ which are at a distance less than $r$ from $x$.*

So, this means that in an open set, every point has a little bubble around it which is also contained in the set.

**Exercise 29.** *Prove that a ball, defined as above,*

$$B_r(x) = \{y \in \mathbb{R}^n \mid |x - y| < r\} \subset \mathbb{R}^n$$

*is an open set.*

Here is a fun thought exercise.

**Exercise 30.** *Draw a "ball" in $\mathbb{R}^1$. Draw a "ball" in $\mathbb{R}^2$. In which dimension, that is $\mathbb{R}^n$ for which $n$, does a "ball" really look like a "ball"?*

We also need the notion of a closed set. To explain this, we first need to fill you all in on what is the complement of a set.

**Definition 4.4.2.** *The complement of a set $S \subset \mathbb{R}^n$ is defined to be*

$$S^c := \mathbb{R}^n \setminus S = \{z \in \mathbb{R}^n \mid z \notin S\}.$$

*That is, the complement of $S$ is the set of all points in $\mathbb{R}^n$ which are* not *in $S$.*

Now, we can define what it means for a set to be closed.

**Definition 4.4.3.** *A set $S \subset \mathbb{R}^n$ is closed precisely when its complement is open.*

**Exercise 31.** *Prove that the set*

$$\overline{B_r(x)} = \{y \in \mathbb{R}^n \mid |x - y| \leq r\}$$

*is closed. (That's why it's called a closed ball, whereas $B_r(x)$ is called an open ball).*

This next exercise is rather intriguing...

**Exercise 32.** *There are precisely two subsets of* $\mathbb{R}^n$ *which are* both *open* and *closed. Which sets are they? (Challenge: prove that these are the only two such sets in* $\mathbb{R}^n$*.)*

The preceding introduction to open and closed sets was required so that we could define *compact* sets.

**Definition 4.4.4.** *A set* $S \subset \mathbb{R}^n$ *is said to be bounded if it fits in a ball. That is, if there exists some* $x \in \mathbb{R}^n$ *and some* $r > 0$ *such that*

$$S \subset B_r(x).$$

*A set which is both closed and bounded in* $\mathbb{R}^n$ *is called* compact.

**Exercise 33.** *Prove that a closed ball,* $\overline{B_r(x)}$ *is compact.*

There is a much more abstract definition, which you'll probably never need in your lives, but just so that you're aware of its existence, here we go.

**Definition 4.4.5.** *A set* $S$ *in a topological space (that's just a space which has a notion of open sets) is compact precisely if every open cover admits a finite subcover.*

Don't worry, we shall not be requiring that definition, nor shall be needing to think about topological spaces. Finally, we can get closer to defining distributions. We're almost there. Distributions are functions which themselves take as input *smooth, compactly supported* functions. So, let's define the input which will go into our distributions.

**Definition 4.4.6.** *A smooth compactly supported function,* $f$*, defined on* $\mathbb{R}$ *(with real or complex values), is a function which is infinitely differentiable, and for which there exists a compact set* $S \subset \mathbb{R}$ *such that*

$$f(x) = 0 \forall x \notin S.$$

We would say that

the function $f$ *lives* on the set $S$.

More precisely, the statement is that "$f$ is supported on $S$." We can think of $f$ as *living* on $S$, because outside of $S$ the function is zero so it vanishes there. Hence, it is never "seen" outside of $S$. So, well, it's living in or on $S$. We denote the set of smooth, compactly supported functions on $\mathbb{R}$ by

$$\mathcal{C}_c^\infty(\mathbb{R}).$$

There is an important norm we can define on these functions, which has a cool name. It is the $\mathcal{L}^\infty$ norm! Some people call it the supremum or sup-norm. It is defined in this way:

$$||f||_\infty = \sup_{x \in \mathbb{R}} |f(x)| = \text{ the maximum value of } |f| \text{ on } \mathbb{R}.$$

The reason that the supremum is equal to the maximum is because the function $f$ lives on a compact set by definition of $\mathcal{C}_c^\infty(\mathbb{R})$. So, since it's smooth, it's also continuous. Moreover, $|f|$ is also continuous. A continuous function on a compact set always assumes a maximum and minimum value. So, $||f||_\infty$ is just the maximum value of $|f|$.

**Definition 4.4.7.** *A* distribution *is a function which maps $\mathcal{C}_c^\infty(\mathbb{R})$ to $\mathbb{C}$, which satisfies the following conditions:*

- *It is linear, so for a distribution denoted by $L$, we have*

$$L(\alpha f + \beta g) = \alpha L(f) + \beta L(g),$$

*for all $f$ and $g$ in $\mathcal{C}_c^\infty(\mathbb{R})$ and for all complex numbers $\alpha$ and $\beta$.*

- *It is continuous in the following sense. If a sequence of functions $\{f_n\}_{n\in\mathbb{N}} \subset \mathcal{C}_c^\infty(\mathbb{R})$ satisfy: there exists a compact set $S \subset \mathbb{R}$ such that all of the $\{f_n\}_{n\in\mathbb{N}}$ are supported on $S$ (they all live in the same compact set) and*

$$\lim_{n\to\infty} ||f_n||_\infty = 0,$$

*and*

$$\lim_{n\to\infty} ||f_n^{(k)}||_\infty = 0,$$

*for all $k$ (where $f_n^{(k)}$ denotes the $k^{th}$ derivative of $f_n$) then*

$$\lim_{n\to\infty} L(f_n) = 0.$$

It may seem like a lot, so let's do some simple examples. The set of distributions is written

$$\mathcal{D}(\mathbb{R}).$$

So, for $L \in \mathcal{D}(\mathbb{R})$, $L$ takes in elements of $\mathcal{C}_c^\infty(\mathbb{R})$ and spits out complex numbers. It satisfies the above properties. Let's do an example.

**Exercise 34.** *Define a distribution in the following way. For $f \in \mathcal{C}_c^\infty(\mathbb{R})$,*

$$L(f) := f(0).$$

*That is, the distribution takes in the function, $f$, and spits out the value of $f$ at the point $0 \in \mathbb{R}$. Show that this distribution satisfies for any $f$ and $g$ in $\mathcal{C}_c^\infty(\mathbb{R})$ and for any $\alpha$ and $\beta \in \mathbb{C}$,*

$$L(\alpha f + \beta g) = \alpha L(f) + \beta L(g).$$

*Moreover, show that if a sequence of functions $\{f_n\}_{n\in\mathbb{N}} \subset \mathcal{C}_c^\infty(\mathbb{R})$ satisfy: there exists a compact set $S \subset \mathbb{R}^n$ such that all of the $\{f_n\}_{n\in\mathbb{N}}$ are supported on $S$ (they all live in the same compact set) and*

$$\lim_{n\to\infty} ||f_n||_\infty = 0, \quad \lim_{n\to\infty} ||f_n^{(k)}||_\infty = 0$$

*for all derivatives of all orders $k \geq 1$ then*

$$\lim_{n\to\infty} L(f_n) = 0.$$

The distribution above is called the *delta* distribution. It is usually written with the letter $\delta$. A whole lot of distributions come from functions which are themselves in $\mathcal{C}_c^\infty(\mathbb{R})$.

**Exercise 35.** *Assume that $f \in \mathcal{C}_c^\infty(\mathbb{R})$. Show that by defining*

$$L_f(g) = \int_{\mathbb{R}} f(x)g(x)dx, \quad g \in \mathcal{C}_c^\infty(\mathbb{R}),$$

*$L_f \in \mathcal{D}(\mathbb{R})$.*

In fact, the assumption that $f \in \mathcal{C}_c^\infty(\mathbb{R})$ wasn't even necessary. You can show that for $f \in \mathcal{L}^2(\mathbb{R})$ or $f \in \mathcal{L}^1(\mathbb{R})$, the distribution, $L_f$ defined above (it takes in a function $g \in \mathcal{C}_c^\infty(\mathbb{R})$ and integrates the product with $f$ over $\mathbb{R}$), is well, yeah, a distribution. So, here's something which is rather cool. The elements in $\mathcal{L}^2(\mathbb{R})$ and $\mathcal{L}^1(\mathbb{R})$ are in general *not* differentiable at all. However, the *distributions* we can make out of them *are* differentiable. Here's how we do that.

**Definition 4.4.8.** *The derivative of a distribution, $L \in \mathcal{D}(\mathbb{R})$ is another distribution, denoted by $L' \in \mathcal{D}(\mathbb{R})$, which is defined by*

$$L'(g) = -L(g'), \quad g \in \mathcal{C}_c^\infty(\mathbb{R}).$$

To see that this definition makes sense, we think about the special case where $L = L_f$, and $f \in \mathcal{C}_c^\infty(\mathbb{R})$. Then, we *can* take the derivative of $f$, and it is also an element of $\mathcal{C}_c^\infty(\mathbb{R})$. So, we can define $L_{f'}$ in the analogous way. Let's write it down when it takes in $g \in \mathcal{C}_c^\infty(\mathbb{R})$,

$$L_{f'}(g) = \int_{\mathbb{R}} f'(x)g(x)dx.$$

We can do integration by parts. The boundary terms vanish, so we get

$$L_{f'}(g) = \int_{\mathbb{R}} f'(x)g(x)dx = -\int_{\mathbb{R}} f(x)g'(x)dx.$$

So,

$$L_{f'}(g) = -L_f(g') = (L_f)'(g).$$

This is why it makes a lot of sense to define the derivative of a distribution in this way. For the heavyside function, we define

$$L_H \in \mathcal{D}(\mathbb{R}), \quad L_H(g) = \int_0^\infty g(x)dx.$$

Then, we compute that

$$L'_H(g) = -L_H(g') = -\int_0^\infty g'(x)dx.$$

Due to the fact that $g$ is compactly supported, it is zero outside of some compact set. So,

$$\lim_{x\to\infty} g(x) = 0.$$

Hence, we have

$$-\int_0^\infty g'(x)dx = -(0 - g(0)) = g(0) = \delta(g).$$

So, we see that the derivative of $L_H$ is the $\delta$ distribution! Pretty neat!

So, now we reach the culmination of this project. Distributions can solve differential equations! For example, we'd say that a distribution $L$ satisfies the equation

$$L'' + \lambda L = 0$$

if, for every $g \in \mathcal{C}_c^\infty(\mathbb{R})$ we have

$$L''(g) + \lambda L(g) = 0.$$

This turns out to be incredibly useful and important in the theory of partial differential equations. However, the way it usually works is that instead of actually finding a distribution which solves the PDE, one shows by abstract mathematics that there *exists* a distribution which solves the PDE. Then, one can use clever methods to show that the mere existence of a distribution solving the PDE, which is called a *weak solution,* actually implies that there exists a genuinely differentiable solution to the PDE. We don't want to get ahead of ourselves here, so conclude with one last exercise, which proves that you can differentiate distributions as many times as you like!

**Exercise 36.** *Verify that if $g \in \mathcal{C}_c^\infty(\mathbb{R})$ then $g'$ is also. Check that if $L \in \mathcal{D}(\mathbb{R})$ then so defined, $L' \in \mathcal{D}(\mathbb{R})$, satisfies the definition of being a distribution. Finally, use induction to show that you can differentiate a distribution as many times as you like, by defining*

$$L^{(k)}(g) := (-1)^k L(g^{(k)}).$$

## 4.5 Project: exercise!

In this project you simply complete the exercises from Chapters 1–3. Moreover, from the Exercises in 3.2.6, you need only do either the odd numbers or the even numbers; your choice! From Exercise 14, you only need to solve 1,3,5,11, and 12.

## 4.6 Project X

Creativity should always be encouraged amongst scientists. Hence, you are welcome to come up with your own project and present it to the instructor of this course for approval. If it is deemed a suitable project, then you can do your own project, which we call Project X.