Partial and (extra)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

$$A + B \to C.$$

(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:

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

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 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:

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

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

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

$$y' = xy$$

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

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

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

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

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

Definition 1.2.2. *Every 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 j^{th} 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. $4x^2 u''(x) + 12xu'(x) + 3u(x) = 0.$
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 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?

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.

Chapter 2

Systems of ODEs

Consider an equation

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

Exercise 7. *Classify the above equation.*

We see that it is a linear, homogeneous ODE with constant coefficients. How can we solve it? Well, if we assume that u is a real analytic function, then we can express it using a power series expansion,

$$u(x) = \sum_{n \geq 0} a_n x^n.$$

We can then substitute this into the equation, and we'll get equations for a_n with $n \geq 3$ which depend on a_0, a_1, and a_2.

Exercise 8. *Substitute*

$$\sum_{n \geq 0} a_n x^n$$

for u in the equation $u''' + 2u'' - u' + 3u = 0$. Use this to determine recursive formulae for the coefficients a_n as described above. Show that if you are given $u(0)$, $u'(0)$, and $u''(0)$, then the solution $u(x)$ is uniquely determined.

The method we used to solve the equation works, but it is a bit tedious. Imagine doing it for an equation which has derivatives up to order 20. It would take a lot of time. Fortunately, someone came up with a clever trick...

2.1 Turning a higher order ODE into a system of first order ODEs

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

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

Let $\lambda \in \mathbb{R}$ and $V \in \mathbb{R}^3$. Consider

$$U = Ve^{\lambda t}.$$

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 λ is the corresponding eigenvalue. Note that for U of this type,

$$U(0) = V.$$

Theorem 2.1.1. *Let M be an $n \times n$ matrix. Then the eigenvalues of M are the roots of the polynomial*

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

where I is the $n \times n$ identity matrix. There are precisely n eigenvalues, counting multiplicity, denoted by λ_1, λ_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 λ, there is at least one vector $V \in \mathbb{C}^n$ with*

$$MV = \lambda V.$$

Actually finding the eigenvalues of a matrix is pretty annoying, and it becomes more and more annoying the larger the matrix is. Fortunately, matrices crop up all over the place, in math, computer science, and everyday purposes (think google), and so there have been many efforts to create efficient software for computing the eigenvalues of matrices. So, the good news is that one must simply put the equation into this form, then 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. 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,

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

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

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

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

Next, we will see how to take the eigenvalues and eigenvectors of M to find all the solutions of the ODE, as well as to find a specific solution if we are provided with sufficient information. We will also consider the general situation of systems of ODE which do *not* necessarily arise from a single ODE.

2.2 Solving systems of ODEs

There are many circumstances in science and engineering which may arise in which we have several functions representing quantities that depend on one another. The simplest example from chemistry is a chemical reaction. 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.

Definition 2.2.1. *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.

We have seen how to turn higher order ODEs into a system of first order ODEs by simply using more unknown functions. On the other hand, we could also begin with a system of first order ODEs for n unknown functions. The way to solve it is precisely the same. 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.

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.

Exercise 10. *Show that if M has real valued matrix entries and $\lambda \in \mathbb{C}$ is an eigenvalue of M, then $\overline{\lambda}$ is also.*

We must now make a subtle distinction. 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. It is in general not very easy to write down what it is. However, we don't need to be able to do that, because we're going to just ask our computers or calculators to find the eigenvalues of the matrix. Here, we are just collecting the facts.

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 λ_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.* Here's where things get a little weird. For each number which appears in the list $\lambda_1 \ldots \lambda_n$, there is at least one eigenvector. There could be more. The number of *linearly independent eigenvectors* is the *geometric multiplicity.* We always have the inequality:

$$\text{geometric multiplicity} \ \leq \ \text{algebraic multiplicity}.$$

Returning to the solutions of the ODE system, we take the eigenvalues and linearly independent eigenvectors. For a real eigenvalue, λ, which is simple (this means its algebraic multiplicity is one), we have a real eigenvector, V, and a solution to the ODE system is

$$Ve^{\lambda t},$$

as well as constant multiples of this,

$$cVe^{\lambda t}, \quad c \in \mathbb{R}.$$

For a real eigenvalue, λ, which has geometric multiplicity k, there are k linearly independent real eigenvectors, V_1, ..., V_k, and solutions with this eigenvalue are

$$\sum_{j=1}^{k} c_j V_j e^{\lambda t}, \quad c_j \in \mathbb{R},\ j = 1, \dots, k.$$

For complex eigenvalues, λ and $\overline{\lambda}$, with corresponding eigenvector V, there are two real solutions,

$$e^{\Re(\lambda)t}\left(\Re(V)\cos(\Im(\lambda)t) - \Im(V)\sin(\Im(\lambda)t))\right),$$

and

$$e^{\Re(\lambda)t}\left(\Re(V)\sin(\Im(\lambda)t) - \Im(V)\cos(\Im(\lambda)t)\right).$$

Recall that the weird script $\Re(\lambda)$ refers to the real part of λ, and the weird script $\Im(\lambda)$ refers to the imaginary part of λ. We shall now turn to a discussion of the general solutions and specific solutions.

2.2.1 General and particular solutions

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. The general solutions for a real eigenvalue, λ, which is simple with eigenvector V,

$$cVe^{\lambda t}, \quad c \in \mathbb{R}.$$

4. The general solutions for a real eigenvalue, λ, which has geometric multiplicity equal to k, are

$$\sum_{j=1}^{k} c_j V_j e^{\lambda t}, \quad c_j \in \mathbb{R},\ j = 1, \dots, k.$$

5. The general solutions for a complex eigenvalue, λ, are

$$ae^{\Re(\lambda)t}\left(\Re(V)\cos(\Im(\lambda)t) - \Im(V)\sin(\Im(\lambda)t))\right) + be^{\Re(\lambda)t}\left(\Re(V)\sin(\Im(\lambda)t) - \Im(V)\cos(\Im(\lambda)t)\right),$$

with a and b real numbers.

6. To find a *particular solution,* one requires additional information. We would need to know
$$U(0) = V_0.$$
Then, we need to check:

7. Is there a simple eigenvalue, λ, with eigenvector, V, and $c \in \mathbb{R}$ with
$$cV = V_0?$$
If yes, then the particular solution we seek is
$$U = cVe^{\lambda t}.$$

8. If no, then we proceed to check the real eigenvalues, λ which have geometric multiplicity $k > 1$, and linearly independent eigenvectors $V_1, \dots, V_k$. Are there real numbers $c_1, \dots, c_k$ such that
$$V_0 = \sum_{j=1}^{k} c_j V_j?$$
If the answer is yes, then the solution we seek is
$$U = \sum_{j=1}^{k} c_j V_j e^{\lambda t}.$$

9. If the answer is no, then we proceed to the complex eigenvalues λ. Are there real numbers a and b such that
$$a\Re(V) - b\Im(V) = V_0?$$
If so, then the solution we seek is
$$U =$$
$$ae^{\Re(\lambda)t}\left(\Re(V)\cos(\Im(\lambda)t) - \Im(V)\sin(\Im(\lambda)t)\right) + be^{\Re(\lambda)t}\left(\Re(V)\sin(\Im(\lambda)t) - \Im(V)\cos(\Im(\lambda)t)\right).$$

2.3 A different perspective

For a higher order, homogeneous, linear ODE with constant coefficients, there is an alternative way to see things. By now, we know that solutions will be something like exponential functions or sines and cosines, which are just exponential functions with complex exponents. So, we could already begin by setting
$$u(t) = e^{\lambda t},$$
and substituting this into the ODE. For example, consider the ODE,
$$u^{(5)} + 3u''' + 2u'' + u' + u = 0.$$

If we assume $u(t) = e^{rt}$, then the ODE is equivalent to finding the solutions, λ, to the polynomial equation,

$$r^5 + 3r^3 + 2r^2 + r + 1 = 0.$$

The same holds if we assume $u(t) = ce^{rt}$ for some constant c. It is a matter of taste, whether one proceeds this way, or whether one turns the higher order ODE into a system. There are advantages to the system method, in that there has been much work done to understand matrices, their eigenvalues, and their eigenvectors. The initial conditions separately, $u(0)$, $u'(0)$, $u''(0)$, $u'''(0)$, and $u''''(0)$, are necessary information to determine a specific solution of a fifth order ODE. With the system method, one deals with all of these simultaneously and determines whether or not there is indeed a solution, by the method above. However, it is good to be aware that for linear, constant coefficient, homogeneous ODEs, one can also proceed by the polynomial method, if that is preferable.

Chapter 3

Techniques for first and second order eODEs

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 11. *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 12. *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

$$\begin{aligned} u_1'(t) &= -0.04u_1 + 10000u_2u_3, \\ u_2'(t) &= 0.04u_1 - 10000u_2u_3 - 30000000u_2^2, \\ u_3'(t) &= 30000000u_2^2. \end{aligned}$$

Exercise 13. *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 coefficient

Is the equation of the form

$$u' - au = b, \quad a \in \mathbb{R}, \quad b \in \mathbb{R}?$$

The solutions in this case are

$$u(t) = ce^{at} - b/a, \quad c = u(0) + \frac{b}{a}.$$

3.2.2 First order linear non-constant coefficients: the Mμthod

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

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

3.2.3 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 Φ 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]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."

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

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

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

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

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

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

3.2.4 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 Ψ 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 Ψ 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.

3.2.5 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 Mμthod.

3.2.6 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.

3.2.7 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

$$c_1 y_1 + c_2 y_2, \quad c_1, c_2 \in \mathbb{R}.$$

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:

$$c_1 e^{rx} + c_2 x e^{rx}.$$

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 15. *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 λ 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 eODE*

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

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. *Let L be the ODE operator,*

$$L(y) = y'' + p(t)y' + q(t)y.$$

Let Y_i be solutions to

$$L(Y_i) = g(t), \quad i = 1, 2.$$

Then $Y_2 - Y_1$ is a solution to

$$L(y) = 0.$$

Therefore, if y_1 and y_2 are a basis for the solutions of the ODE $L(y) = 0$, then for every pair of solutions to the inhomogeneous ODE

$$Y_2 - Y_1 = c_1 y_1 + c_2 y_2, \quad c_i \in \mathbb{R}, i = 1, 2.$$

Theorem 3.3.3. *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

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

Here are a few exercises to try:

Exercise 16. *Solve the following equations:*

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

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

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

Exercise 18. *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 α, β, and all the way up to Γ in terms of a, b, c, d, e, f, g together with the partial derivatives of the coordinates η and ξ.

Exercise 19. *Set the coefficients α and γ 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 ξ, and B be a root of the equation for η. Show that

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

will satisfy the equation.

Exercise 20. *Write up the PDE in terms of the coordinates ξ and η, and verify that indeed it only contains one second derivative, $u_{\xi\eta}$.*

Exercise 21. *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 ξ and η, so that the equation takes the form

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

Exercise 22. *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 α, β, and all the way up to Γ in terms of a, b, c, d, e, f, g together with the partial derivatives of the coordinates η and ξ.

Exercise 23. *The goal now is to set β and either α or γ equal to zero and solve for η and ξ. Do this and determine an equation for either ξ_x/ξ_y or η_x/η_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 ϵ 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 Δ 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 24. *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 25. *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 26. *Using separation of variables, show that (up to a constant multiple) the* Θ *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 27. *Show that* R *must satisfy*

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

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 28. *Show that the equation becomes*

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

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 29. *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 ν is an *integer.* This means that when ν 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 ν, 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 30. *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 31. *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 32. *Prove that the set*

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

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 33. *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 34. *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 α and β.

- *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 35. *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 α 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 δ. A whole lot of distributions come from functions which are themselves in $\mathcal{C}_c^\infty(\mathbb{R})$.

Exercise 36. *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 δ 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 37. *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: two roads to the same answer

In this project, you complete Exercise 8 from Chapter 2. Then, using the method of Chapter 2, turn the equation from Exercise 8 into a system of ODEs. Solve it according to that method. Show that the solution you get, either way, is in fact the same.

4.6 Project: exercise!

In this project you simply complete the exercises from Chapters 1–3, except Exercise 8. Moreover, from the Exercises in 3.2.7, 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.

4.7 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.