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Differential equations and some of their applications in chemistry

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1 Preface

When applying for my thesis, I was unsure of what I wanted to research and write about. When trying to decide what thesis to apply for, I looked for a supervisor I recognised. In hindsight I'm very glad I emphasized who the supervisor was, despite choosing a task I knew absolutely nothing about.

The thesis I applied for was on conformal mapping. Since it turned out I didn't have the needed background knowledge, my supervisor, Alexander Rashkovskii, was kind enough to give me an alternative thesis that I could choose if I wanted. I am very thankful for this unsolicited kindness. It gave me the opportunity to research a topic highly relevant to my subjects this year. It created a red thread through this semester and complimented the subject MAT 320 on Differential equations nicely. So, thank you very much Alexander for your help and guidance.

2 Summary

This thesis gives insight in the big subject of differential equations and its applications in a variety of fields. It is focused on the applications in chemistry, and gives an extensive example of this, and briefly mentions some of the many other applications differential equations have.

Our knowledge of differential equations grew rapidly and the text covers some of the history from the first hundred years.

Lastly, it's given an overview, with simple examples, of some of the many ways to solve and use differential equations.

3 Introduction

Isn't it ironic that the one constant thing, through the history of the universe, is the existence of change? Change has been persistent since before the beginning. Change is the cause of our existence. And where there's change, there are differential equations.

The thesis is based on Boyce's Elementary differential equations and boundary value problems by William E. Boyce, Richard C. Diprima and Douglas B. Meade [5]. It will give a short account for the history of differential equations, convey some general knowledge about differential equations, show some of its applications in chemistry and briefly mention how it's being used in other fields.

4 Historical background

We can thank several different people on the first contributions to the topic of differential equations and the findings of their applications. It took them a century, from 1675 to 1775, not only to discover differential equations, but to find the general methods of differentiating ordinary differential equations. History shows that there were nine different mathematical problems that were the origin of what we now know as ordinary differential equations.

The beginning of our story is believed to date back to November 11th 1675, when Gottfried Wilhelm von Leibniz (1646-1716) wrote:

$$\int y dy = \frac{1}{2}y^2 \tag{1}$$

The discipline of differential equations originates in Isaac Newtons (1643-1727) and Gottfreid Leibniz's studies of calculus. Two independent studies published by Newton in 1687 and by Leibniz in 1684 were the start of this branch of mathematical studies. Although Newton didn't do very much work on differential equations, he identified three different forms of first-order differential equations:[2]

$$dy/dx = f(x) \tag{2}$$

$$dy/dx = f(x, y) \tag{3}$$

$$x\delta u/\delta x + y\delta u/\delta y = u \tag{4}$$

The first two equations represent classes of ordinary derivatives. Here we have one or more dependent variables, with respect to one independent variable. Today these equations are known as ordinary differential equations, and often referred to as ODEs. The latter equation includes the partial derivatives of a single dependent variable and is called a partial differential equation or PDE

Leibniz published two different papers during the 1680s. He was the co-founder of a journal called Acta Eruditorum. The journal consisted of many important papers on several different subjects, such as medicine, mathematics and natural sciences. The first one was published in 1684 and it was a six-page paper on differential calculus [3]. Two years later, in 1686, he published another paper. This one containing the rudiments, or the basics, of integral calculus [4]. Leibniz was the first to use the notation of the integral sign that we use today.

Another name that comes up when studying differential equations is Bernoulli. The brothers, Jacob (1654-1705) (also known as James) and Johann Bernoulli (1667-1748), were both mathematicians and their contributions to the study of differential equation is remarkable. Jacob, while working as a professor at the University of Basel, wrote to Leibniz and asked for insight on the calculations Leibniz had done in his papers. Due to traveling Leibniz didn't answer Jacob Bernoulli for three years.

In the meantime, Jacob and Johann worked together to find out the mystery of Leibniz's theories. They were among the first mathematicians to try to understand what Leibniz wrote. When they succeeded it led to a substantial correspondence with Leibniz. Their understanding of calculus and their abilities to use its applications, made the Bernoulli bothers' contributions unparalleled [5, p. 7].

In 1690, Jacob Bernoulli, published his solution to **the isochrone problem** in *Acta Eruditorum*. The isochrone problem is equal to the tautochrone problem, which is explained further down in the text, and it involves an isochronous curve on which an object will fall with vertical velocity. The solution showed a differential equation that state the equality of two differentials.

Leibniz's main contribution to the study of differential equations is dated to 1694. With help form John Napier's work on logarithms, he was able to solve **the problem of the quadrature of the hyperbola** - a process of finding a square equal in area to the area under the curve on a given interval [8]. He did this after an extensive correspondence with Johann Bernoulli, discussing the inversive problem of tangents.

In 1696, Johann Bernoulli, posed **the brachistochrone problem** [7]. He created the problem in order to set himself apart from his brother. They were often quarrelling and there were a lot of jealousy between them [5, p. 7]. The problem, however, was the source of their most bitter dispute. This was due to the fact that they both proposed the same solution, noting that it was the same curve as the tautochrone curve, but Johanns derivations was wrong. In the end five mathematicians gave their solutions: Newton, Liebniz, l'Hôpital, von Tschirnhaus and Jacob Bernoulli. Johann published four of the solutions (excluding l'Hôpital) alongside his own solution.

Later, in 1698, Johann solved **the problem of determining the orthogonal trajectories** of a one-parameter family of curves - finding a curve which cuts all the curves of a family of curves at right angles [8].

Now at the end of the 17th - century, all known elementary methods to solve 1st order differential equations had been found.

Johann Bernoulli was the father of Daniel Bernoulli (1700-1782) and Leonhard Eulers (1707-1783) teacher. The son, Daniel, was both a mathematician and a physicist. He is known for his contributions in both mathematics, physics, economics and statistics. Daniel and Leonhard were friends and study-partners. They worked together to find out more about fluids, and how they move. Bernoulli was given credit for discovering the basis for the kinetic theory of gasses as well as much more. It is also his name that we associate with the Bernoulli equation in fluid mechanics [5, p.7].

The 18th – century took the study of differential equations to new heights. In 1701, Jacob Bernoulli, published the solution to **the isoperimetric problem** - a problem where it is required to make one integral a maximum or minimum while keeping constant the integral of a second given function. This gives a differential equation of the 3rd order.

The next big development was made by Euler in 1728. One of his biggest contributions to the studies of differential equations was solving **the problem of reducing 2nd order equations to 1st order equations** by finding an integrating factor.

Euler was more than just a mathematician. He was a physicist, engineer, astronomer, geographer and logician. His study on complex analysis and analytical number theory was groundbreaking. A lot of the mathematical notation we use today, is also credited Euler.

He also worked with Joseph-Louis Lagrange (1736-1813) and together they made further progress on solving differential equations. The Euler-Lagrange equations are a system of 2nd order ODEs used in classical mechanics and in the calculus of variation [5, p. 14]. These equations were discovered when the Swiss Euler and the Italian Lagrange were studying the tautochrone problem. A few years after Johann Bernoulli had posed the brachistochrone problem, Jacob, made a more complicated version in another attempt to outdo his brother. In his attempt on solving the new problem, he developed new methods that were the cause of Euler's studies on the matter years later. He refined Jacob Bernoulli's methods and applied it when corresponding with Lagrange on the tautochrone problem, which then gave the base for what Euler himself called the calculus of variation.

The tautochrone problem was studied by many different scientist and mathematicians. It is the problem of finding a curve where you can fix several objects in different height on the curve, letting gravity work without friction, and they arrive at the bottom at the same time. The problem was solved in 1659 by Chrisitaan Huygens (1629-1695) [6].

Lagrange solved this problem, and then sent it to Euler, how helped refine and further develop his methods. Later they applied it to mechanics, which then led to the composition of Lagrangian mechanics.

A new name arises when Alexis Claude Clairaut (1713-1765) applied the process of differentiation to this equation:

$$y = xdy/dx + fdy/dx$$

The equation is known today as the Clairaut's equation. Clairuat published his work on this class of equations in 1734 [8]. Clairaut was also one of the first to solve **the problem of singular solutions** - finding an equation of an envelope of the family of curves represented by the general solution.

Lagrange formalized the concept of the adjoint equation, while he worked on **the problem of determining an integration factor for a general linear equation** in 1743. He also showed that the general solution of a homogeneous linear equation of nth order is a linear combination of n independent variables. Later, in 1774-1775, he discovered the method of variations of parameters [5, p.14].

In 1762, Jean Le Rond d'Alembert (1717-1783), building on Lagrange's work, found the conditions under which the order of a linear differential equation could be lowered [8]. He solved **the problem of linear equations with constant coefficients**. This later triggered the study of linear differential systems.

By 1775, the discovery of general methods to integrate ordinary differential equations ebbed out. The new problems that appeared, needed more sufficient methods with special properties. The study of functions with boundary value problems and criteria that could guaranty the existence of a solution, led to a more analytical approach. But now we can see that it was the solutions of these nine problems (marked in bold) that laid down the foundation for mathematical discipline of solving differential equations.

4.1 Why differential equations are still important today

We have now reviewed the quite explosive start of the history of differential equations. The first hundred years were packed with developments, applications and lots of new information on the subject. The reason this particular part of the mathematical history is so dense, is that the mathematicians saw that differential equations opened up a whole new possibility of explanations.

It has been stated, that differential equations are used for describing change. They are tools for modelling certain situations and can be used in a variety of fields. As far as physics, chemistry and engineering goes, nearly all of the 'general' laws are expressed using differential equations. Some examples are Newton's law of cooling, Newton's law of motion, fluid dynamics equations, Maxwell's equations, equations in stellar dynamics and in plasma dynamics, Hook's law, acoustic wave equation, equations in chemical kinetics and in thermodynamics, Schrödinger's equation, Einstein's equation for general relativity and the list goes on and on. It is seemingly endless in both variety and length.

It is also useful to know that differential equations are often the briefest, or most succinct, way of describing and defining a function. Differential equations characterize functions in operationally meaningful ways. They tie together different branches of mathematics, one might else think of as separate and it is a manageable study that teaches many methods of exact calculations. Therefore, differential equations are still important today.

5 General knowledge about DEs

We are now in the mathematical field of change, and the rate of change are expressed by derivatives. We use calculus to set up an equation with an unknown function and it derivative $y = f(x)$. This is known as a differential equation. There are many different techniques for solving such equations. We can calculate direct solutions, use a graph, or do calculations using a computer.

5.1 General differential equations

Differential equations always include a derivative. A simple example of what a differential equation can look like could be $y' = 3x^2$. There is a relationship between the variables x and y, where y is a function of x, and therefore it varies with x. We can find a solution to this equation if we start by imagining that we have a function $y = f(x)$ and finding its derivative. The derivative must be equal to $3x^2$. Now what function has a derivative equal to $3x^2$? One such function is $y = x^3$. This function is now considered a solution to the differential equation.

Definition 5.1. A *differential equation* is an equation involving an unknown function $y = f(x)$ and one or more of its derivatives. A solution to a differential equation is a function $y = f(x)$ that satisfies the differential equation when f and its derivatives are substituted into the equation.

We note that a solution to a differential equation may not be unique. That is because the derivative of a constant is zero. Therefore $y = x^3 + 5$ could also be a solution to the previous differential equation. There are different characteristics we can look for or define to separate and categorize differential equations. The most basic characteristic is the order of the differential equation.

Definition 5.2. The *order* of a differential equation is the highest order of the derivative of the unknow function that appears in the equation.

Example 5.3.

$$y\prime = xy, y = y(x) \rightarrow \text{1st order}$$

$$x\prime\prime = xx\prime + 2t, x = x(t) \rightarrow \text{2nd order}$$

$$uxx = utt, u = u(x,t) \rightarrow \text{2nd order}$$

We can also characterize differential equations by whether they are ordinary or partial, linear or nonlinear, homogeneous or nonhomogeneous, and more.

Not all differential equations are solvable. But for those how are, we can most often find both a general and a particular solution. We have already seen that the $y' = 3x^2$ has two solutions: $y = x^3$ and $y = x^3 + 5$. The only difference is the last constant. In fact, the last constant can be anything. Therefore, we can denote it as C and write $y = x^3 + C$ as a solution to the equation. This is what we call a **general** solution to an equation. Note that linear differential equations are easier to solve than nonlinear, but they can still have infinitely many solutions. There is no restriction for C, but in the example given in figure 3.1, I've used integer values. The figure shows a family of solutions to the equation $y' = 3x^2$.

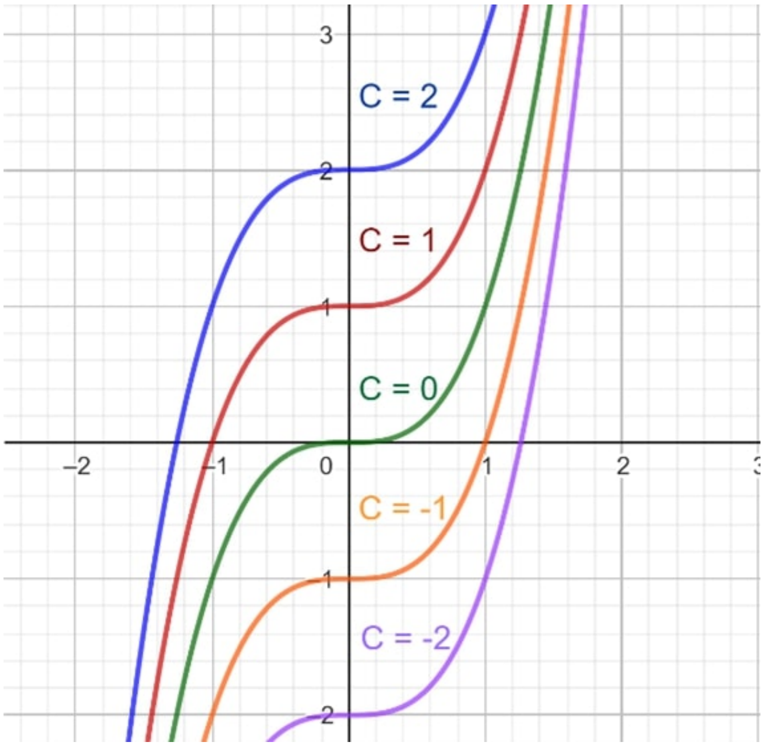

Figure 1:

In order to find a particular solution, we need eighter a point the graph goes through, or some initial conditions (ICs). If we have a differential equation with initial conditions, we call it an initial-value problem (IVP). These we can solve for C and get a particular solution. If we have an IVP of higher order than one we need more initial conditions to be able to solve for a particular solution. So we can see that when we have a general solution, we get a family of functions. These functions can be explicit – defined by a formula, or implicit – defined by an equation. The initial value(s) determine which of the solutions that satisfies the wanted conditions.

6 General applications of DEs

Differential equations describe how nature works. That's why they are so important and known by all kinds of physicists, chemists, biologists, mathematicians, economists, engineers, builders and so many others. Mankind have always wondered how the universe works in all its wonders, and the answer is in short: differential equations.

There are many different examples of how differential equations are used in the real world. Modelling how a population grows involves differential equations. How any fluid moves: differential equations. Electromagnetism, which is how phones, radio Wi-Fi and GPS all work: four differential equations known as the Maxwells equations. Electric circuits, and even if something touches something else, and thus exerts a force, differential equations are used to describe the motion. Even if there's no physical contact, like with orbiting bodies, there is still a force so there's still differential equations.

Now, say that we want to get a deeper understanding of our own personal economy, and we take a look at one of our bank accounts. We want to write a differential equation that describes, or models, the change in the bank account.

First we start by letting $y(t)$ represent the bank account balance, in kroner, after t years. Suppose we start with $100000kr$ in the account. Each year the account earns 3% interest, and I withdraw $6000kr$.

If $y(t)$ represent the bank account balance, in kroner, after t years, then $y'(t)$ or $\frac{dy}{dt}$ will be the change in the amount of kroner with respect to time. There are two things that affect the account balance. It is the 3% interest that increases the balance, and the $6000kr$ withdraw the decreases the balance. So, if we put this in mathematical terms we get an equations like this:

$$\frac{dy}{dt} = 0.03y - 6000 \tag{5}$$

The differential equation measures the change in the account balance per unit of time, the time being measured in years. We also have that $y(0) = 100000$ as an initial condition. Now we want to solve for $y(t)$. So, we're going to star of by finding the general solution using the method of substitution of variables, and then use the initial condition to find a particular solution. First, we're going to rearrange the terms so that we get the y-terms on one side of the equation, and the t-term on the other.

$$\frac{dy}{dt} = 0.03y–6000$$

$$dy = (0.03y – 6000)dt$$
$$\frac{1}{0.03y - 6000} dy = dt$$

Let's take the integral on both sides of the equation.

$$\int \frac{1}{0.03y - 6000} dy = \int dt$$
$$\frac{ln|0.03y - 6000|}{0.03} = t + C_1$$
$$C = C_1 * 0.03$$
$$ln|0.03y - 6000| = 0.03t + C$$
$$0.03y - 6000 = e^{0.03t} * e^C$$
$$A = e^C$$
$$0.03y - 6000 = Ae^{0.03t}$$
$$y(t) = \frac{Ae^{0.03t} – 6000}{0.03}$$

Now we have a general solution to our problem: $y(t) = \frac{Ae^{0.03t} – 6000}{0.03}$. By using our initial condition, we can find a particular solution by solving for A.

$$100000 = \frac{Ae^0 – 6000}{0.03}$$
$$3000 = A – 6000$$
$$A = 9000$$
$$y(t) = \frac{9000e^{0.03t} – 6000}{0.03}$$

This is our final product, a particular solution that we can use to monitor our personal economy.

7 Strategies for solving DEs and how to use them

Since there are many different types of differential equations, and they may have many different characteristics, there are also many different ways of solving them. It is only the simplest equations that can be solved explicitly; however, many properties of their solutions can be determined without solving them exactly.

The different types of differential equations are not only helpful for classifying or differentiating them, but they can also help us decide how to approach the solution. The most common ways to distinguish the differential equations are whether or not they are ordinary or partial, homogeneous or heterogeneous, linear or non-linear, which order or degree it has and many more. There are other properties and subclasses that can be useful in specific contexts.

Having already stated that not all differential equations can be solved exactly, it might be interesting to look at what it means to 'solve' a differential equation. If we're asked to solve a differential equation, we need to find all functions which satisfy the differential equation when substituted for the unknown function(s). This is called a general solution. We saw in chapter 3 that we need one or more initial conditions to be able get a particular solution.

Before we start trying to solve a differential equation, it will be interesting to know if the differential equation has a solution. Unfortunately, not all differential equations have a function that satisfies it. When questioning the existence of a solution, we have theorems stating that under certain restrictions or assumptions on the differential equation, the equations always have solutions. Verifying the existence of a solution is not only a theoretical concern. If a problem doesn't have a solution, it would be preferable to know that before putting time and effort in a vain attempt to solve the problem. In a situation where the problem is a sensible, physical problem modelled by a differential equation, then we would expect it to have a solution. If it doesn't, then there is presumably something wrong with the formulation. Finding out if the problem has a solution, is a way for physicist or an engineer to check the validity of the model.

Having checked that the problem has a solution, the next thing we need to clarify is how many solutions it may have. We might need to specify additional conditions to single out a particular solution or family of solutions. This is the question of uniqueness. Since solving differential equations requires the use of integration, the solutions generally contain one or more arbitrary constants of C. This means that an equation may have infinitely many solutions due to the value of C. If we find a solution to a problem, and we know that the solution is unique, we can be sure that the problem is completely solved. In a situation where we know that the solution is not unique, we may have to search for other solutions.

Lastly we should know that even if a differential equation has a solution, we may not be able to determine it. We usually express solutions in terms of elementary functions such as polynomial, exponential, logarithmic, trigonometric, and hyperbolic functions. Alas, it is often the case that our solution is not expressible in these terms. In those situations there are methods we can use to obtain exact solutions in relatively simple cases, and more general methods used to find approximations to solutions of a more difficult nature.

Now, if we form here on forth assume that we are to solve problems with an expressible solution, there are several different ways to do so:

7.1 Separation of variables

This method can be used when all y-terms and all x-terms can be separated and put on separate sides of the equation. The process is applicable to a large class of both linear and nonlinear differential equations. The general first-order equation is

$$\frac{dy}{dx} = f(x)g(y) \tag{6}$$

We have that if $g(y_0) = 0$, then $y = y_0$ is a constant solution. But, if $g(y) \neq 0$ we can use substitution and write $h(y) = \frac{1}{g(y)}$ and the differential equations as

$$f(x) = h(y)\frac{dy}{dx} \tag{7}$$

Next step is to integrate on both sides.

Example 7.1.

$$\frac{dy}{dx} = 2xy^2$$

Here we have that if $y^2 = 0$, then $y = 0$ is a constant solution. If $y^2 \neq 0$ we divide the differential equation by y^2 and integrate:

$$\int \frac{dy}{y^2} = \int 2xdx$$

$$-\frac{1}{y} = x^2 + C, \quad \text{implicit form}$$

$$y = \frac{-1}{x^2 + C}, \quad \text{explicit form}$$

7.2 First-order linear differential equation

When solving a first-order linear differential equation, we use the method of integrating factors. An equation is only linear if it fits this form:

$$\frac{dy}{dx} + P(x)y = Q(x) \tag{8}$$

Where P(x) and Q(x) are functions of x.

Note that an equation is only first-order as long as it doesn't contain terms of $\frac{d^2y}{dx^2}$ or $\frac{d^3y}{dx^3}$, etc.

We will explore this method in an extensive example in the next chapter. Therefore, I will not elaborate any further.

7.3 Homogeneous equations

Generally we have that an equation f is called homogeneous if $f(x, y) = f(ax, ay)$ for all $a \neq 0$. A homogeneous equation does not depend on x and y separately, but rather the ratio $\frac{y}{x}$ or $\frac{x}{y}$. Homogeneous equations are written on the form

$$\frac{dy}{dx} = F(\frac{y}{x}) \tag{9}$$

If a first-order differential equation is homogeneous, we can solve the DE using a method of separation of variables, if we first preform a substitution $v = \frac{y}{x}$ or $y = vx$, and $\frac{dy}{dx} = x\frac{dv}{dx} + v$. Then we solve the original differential equation in terms of x and y.

Example 7.2. Determine whether the following differential equations are homogeneous. If homogeneous, then solve.

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

For this equation to homogeneous, we need to see if we can write the right side of the equation as a function of $\frac{y}{x}$. The first thing we do is rewrite the right side by multiplying both the denominator and the numerator by $\frac{1}{x^2}$. Looking at the denominator we see that it simplifies to 1, and the nominator we get $3(\frac{y}{x})^2 + \frac{y}{x}$. Now we see that the right side of the equation is a function of $\frac{y}{x}$. Therefore, we know that this is a homogeneous differential equation, and we can solve it by using the substitutions mentioned earlier.

Performing the substitution, we get:

$$x\frac{dv}{dx} + v = 3v^2 + v$$

Now we can subtract v on both sides and move the $x - terms$ to the right-hand side before we integrate on both sides of the equation.

$$\int \frac{1}{3}v^{-2}dv = \int \frac{1}{x}dx$$

The integration then gives us an equation that we're going to rewrite in terms of x and y.

$$-\frac{1}{3}v^{-1} = \ln|x| + C$$
$$\frac{x}{y} = -3\ln|x| - 3C$$

Substituting $-3C$ for C_1, we now solve for y.

$$y = \frac{x}{C_1 - 3\ln|x|}$$

This is our general solution to the original homogeneous differential equation.

7.4 Bernoulli equations

Bernoulli equations are on the general form:

$$\frac{dy}{dx} + P(x)y = Q(x)y^n$$

Where n represents any real number except 0 and 1.

When $n = 0$ the equation can be solved as a first-order linear equation, and when $n = 1$ it can be solved by separation of variables. For other values of n, we can solve by substituting $v = y^{1-n}$ and turn it into a linear equation, and solved it as such. After solving for v, we can determine the solution to the original differential equation, which will be to solve for y.

Example 7.3. Solve the Bernoulli equation.

$$y\prime + xy = xy^2$$

First we notice that we have $n = 2$. This gives us $v = y^{-1} = \frac{1}{y}$, which in turn lets $y = \frac{1}{v} = v^{-1}$. Next $y\prime = -v^{-2}\frac{dv}{dx}$. Now we can go ahead and preform the substitution.

$$-v^{-2}\frac{dv}{dx} + xv^{-1} = xv^{-2}$$

This is now a linear first-order equation, which we can solve for v. First, we need the equation on linear form in order to determine the integrating factor. Dividing each term by $-v^{-2}$, we get:

$$\frac{dv}{dx} - xv = -x$$

Remembering from the section on linear equations, we need it on the form $\frac{dy}{dx} + P(x)y = Q(x)$. Where we use $P(x)$ to decide the integration factor $\mu(x) = e^{\int [P(x)]dx}$. In this case we have $P(x) = -x$, so the integrating factor will be $\mu(x) = e^{-\frac{x^2}{2}}$. Multiplying this with each term in the equation we get:

$$e^{-\frac{x^2}{2}}\frac{dv}{dx} - xe^{-\frac{x^2}{2}}v = -xe^{-\frac{x^2}{2}}$$

The left-hand side is equal to the derivative of the product of the integrating factor and v.

$$\frac{d}{dx}[e^{-\frac{x^2}{2}}v] = -xe^{-\frac{x^2}{2}}$$

Taking the integral on each side we solve this equation for x, and then we can go back and solve the original equation for y.

Having done the integral and cleaned up the equation a bit, we have that:

$$v = 1 + Ce^{-\frac{x^2}{2}}$$

Looking back at the example we see that we had $v = \frac{1}{y}$ or $y = \frac{1}{v}$. Solving for y we get the answer to the original Bernoulli equation:

$$y = \frac{1}{1 + Ce^{-\frac{x^2}{2}}}$$

7.5 Second-order equation

Second-order, homogeneous equation looks like this:

$$\frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y = 0 \tag{10}$$

If the equation does not equal 0, but rather another function $f(x)$, it is no longer homogeneous. Non-homogeneous second-order DEs can be solved by using different kinds of methods. Firstly, we can use the method of undetermined coefficients if $f(x)$ is a polynomial, exponential, sine or cosine function or a linear combination of those. Secondly, we can use variation of parameters which might be a bit messier, but it works with a wider range of functions.

When the equation is homogeneous, we can substitute y for e^{rx}. When we do this, and we move e^{rx} outside the parentheses, we get a quadratic equation or a characteristic equation, which we can solve by using the quadratic formula. We know that when we use the formula, we can get three different outcomes. There might be two real roots, one real root or two complex roots, which will be our value of r. All these three outcomes, gives dissimilar ways to further solve the equation.

We're going to look at an example of how to solve a homogeneous second-order differential equation with two distinct real roots. The methods of undetermined coefficients and variation of parameters will be covered later.

Example 7.4. Before we look at the equation we're solving, lets note that $P(x)$ and $Q(x)$ will be constants, not functions of x. This will give us an equation that looks like this:

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

The equation we'll be solving is this:

$$y'' - 4y = 0$$

Here we have that $a = 1$, $b = 0$ and $c = 4$. Rearranging the equation, we see that we are looking for a function such that the second derivative is four times the original function. So, we have a function that when twice derivated, it gives us back the original function plus a constant. Using what we know about derivation rules, we see that it will be natural to look at an exponential function. If we let $y = e^{2x}$ we have to apply to chain rule twice to find the second derivative. Doing that we get $y'' = 4e^{2x}$. Now we have a second derivative that is four times the original function. This gives us one solution to our differential equation. There are also many other, but let's look at a second option where $y = e^{-2x}$. Derivating this twice gives us $y'' = 4e^{-2x}$, which again is four times this original function.

To find the general solution to this equations, we're going to apply a principle called *the principle of superposition*. This principle states that if $y_1(x)$ and $y_2(x)$ are two solutions to a linear, homogeneous second-order differential equation, then $y(x) = c_1y_1(x) + c_2y_2(x)$ will be the general solution. In our case it is logical to think that the solution will be exponential, and for such cases we have that $y(x) = c_1e^{r_1x} + c_2e^{r_2x}$. Let's apply this to our problem.

We have $y_1 = e^{2x}$ and $y_2 = e^{-2x}$. We can now use the principle of superposition to find our general solution:

$$y(x) = c_1e^{2x} + c_2e^{-2x}$$

Now we're going to use the method of the characteristic equation to find the general solution to the differential equation. As a reminder, we have already seen that we have $a = 1$, $b = 0$ and $c = 4$ in our original function. Our characteristic equation will then be:

$$r^2 – 4 = 0$$

Using the quadratic formula we solve this for r, which gives us:

$$(r - 2)(r + 2) = 0$$

$r_1 = 2$ and $r_2 = -2$. Now that we know the values of r, we can notice how we have two distinct real roots, which means that our solution will be in the form we saw earlier $y(x) = c_1e^{r_1x} + c_2e^{r_2x}$. This gives the solution:

$$y(x) = c_1 e^{2x} + c_2 e^{-2x}$$

As a sidenote, we can have a brief look at what we would in the cases of one real root and two complex roots. If $r_1 = r_2 = r$, we have one real root. Then $y(x) = c_1 e^{rx} + c_2 x e^{rx}$. If r_1 and r_2 are two complex roots $\alpha \pm \beta i$, then $y(x) = c_1 e^{\alpha x} \cos \beta x + c_2 e^{\alpha x} \sin \beta x$.

7.6 Undetermined coefficients

The method of undetermined coefficients is used when solving non-homogeneous second-order differential equations:

$$\frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y = f(x) \tag{11}$$

$f(x)$ can both be a single function or a sum of two or more functions. To keep thing simple we will look at an example where both $P(x)$ and $Q(x)$ are constants. To find a complete solution for such an occasion we'll need to combine both the homogeneous solution, which we find by putting the equation equal to zero, and the non-homogeneous solution, which is where the equation is equal to the function $f(x)$.

$$Homogeneous: \frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y = 0$$

$$Non \quad homogeneous: \frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y = f(x)$$

The answer to the homogeneous equation gives us the two first terms of our general solution, also called y_c, whilst the answer to the non-homogeneous equation provides the last term, Y_p.

$$General \quad solution: y(x) = c_1 y_1 + c_2 y_2 + Y_p(x)$$

In order to find the complete general solution, we have to make a guess on a particular solution with undetermined coefficients after having solved the homogeneous equation. Then, lastly, we must make a substitution into the original equation and solve for the undetermined coefficient to find the general solution.

Example 7.5. Determine the solution to $y\prime\prime + 2y\prime – y = x^2 - 5x + 6$.

Here we have a non-homogeneous linear differential equation, where $f(x)$ is a polynomial function. First, we want to solve the homogeneous equation and find the complementary function: y_c.

$y\prime\prime + 2y\prime – y = 0$

We recognize that the coefficient are constants, with a differential equation that fits a characteristic equation. Note that $a = 1$, $b = 2$ and $c = -1$, which gives the characteristic equation $r^2 + 2r - 1 = 0$. So, we can solve this by using the quadratic formula we've used before. This gives $y_c = c_1e^{(-1+\sqrt{2})x} + c_2e^{(-1-\sqrt{2})x}$. So far, our general solution looks like this:

$y(x) = c_1e^{(-1+\sqrt{2})x} + c_2e^{(-1-\sqrt{2})x} + Y_p$

In the original equation, we see that $f(x) = x^2 - 5x + 6$, which is a quadratic function. So now, as our step two, we need to guess at a particular solution Y_p. Since $f(x)$ is a quadratic function, then our guess at Y_p, will also be a quadratic function.

$Y_p = Ax^2 + Bx + C$

Next will use this function, with its first and second derivatives, and substitute it for y in the original equation.

$Y_p = Ax^2 + Bx + C$, $Y_p\prime = 2Ax + B$ and $Y_p\prime\prime = 2A$. Now lets preform the substitution.

$2A + 2(2Ax + B) - (Ax^2 + Bx - C) = x^2 - 5x + 6$

Rearranging the equation, we get: $-Ax^2 + (4A - B)x + (2A2B - C) = x^2 - 5x + 6$

Next, we can set up a system of equations and solve for A, B and C - a process called equating coefficients. This gives us $A = -1$, $B = 1$ and $C = -6$. Now that we know the values of A, B and C, we have found the coefficients of our particular solution. Since we know the value of Y_p, we now have the complete general solution to our original equation.

$y(x) = c_1 e^{(-1+\sqrt{2})x} + c_2 e^{(-1-\sqrt{2})x} - x^2 + x - 6$

7.7 Variation of parameters

This method is used in the case of solving a non-homogeneous second-order differential equation. We've already seen examples of how to solve a homogeneous second-order DE and how to use the method of undetermined coefficients. We use variation of parameters when we're dealing with a function that's neither polynomial, exponential, sine or cosine function or a linear combination of those.

The first part of the general solution is found, as in the former case, by solving the equation as if it was homogenous. The rest is found by calculating something called the Wronskian and then using integration. The problem with this method is that, although it may be operative with a wider variety of functions, it can leave us with a solution that contains an integral.

To find the general solution using this method we go through three steps. First, we solve $\frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y = 0$ to find y_c. Step number two, is to find Y_p using this formula:

$$Y_p(x) = -y_1 \int \frac{y_2 g(x)}{W(y_1, y_2)} dx + y_2 \int \frac{y_1 g(x)}{W(y_1, y_2)} dx \tag{12}$$

This formula is derived using the Cramer's rule and it contains the Wronskian, $W(y_1, y_2)$, which is the determinant of the matrix:

$$W = \begin{bmatrix} y_1 & y_2 \\ y_1\prime & y_2\prime \end{bmatrix}$$

So, $W(y_1, y_2)$ is calculated by taking $y_1 y_2\prime - y_2 y_1\prime$. y_1 and y_2 are the answers we get when finding y_c. Step number three is to form the general solution $y(x) = y_c + Y_p = c_1 y_1 + c_2 y_2 + Y_p$.

Example 7.6. Solve $y\prime\prime - y\prime - 2y = e^{3x}$ using variation of parameters.

Step one, we're going to solve the corresponding homogeneous differential equation.

$y\prime\prime - y\prime - 2y = 0.$

Because we have constant coefficients, we can solve this using a characteristic equation where $a = 1$, $b = -1$ and $c = -2$. This gives us, $r^2 - r - 2 = 0$ which we solve by factoring: $(r-2)(r+1) = 0$. This then gives us $r = 2$ and $r = -1$ as the values of r. Since we have two distinct real roots, we get $y_c = c_1e^{2x} + c_2e^{-x}$. We notice that $y_1 = e^{2x}$ and $y_2 = e^{-x}$.

Step two, is to find Y_p using this formula

$Y_p(x) = -y_1 \int \frac{y_2 g(x)}{W(y_1,y_2)} dx + y_2 \int \frac{y_1 g(x)}{W(y_1,y_2)} dx$.

Let us begin by finding the Wronskian of y_1 andy_2.

$$W(y_1, y_2) = \begin{bmatrix} e^{2x} & e^{-x} \\ 2e^{2x} & -e^{-x} \end{bmatrix}$$

Calculating this we get $W(y_1, y_2) = -3e^x$. Now we can go ahead and find Y_p. $Y_p(x) = -e^{2x} \int \frac{e^{-x}e^{3x}}{-3e^x} dx + e^{-x} \int \frac{e^{2x}e^{3x}}{-3e^x} dx$

Cleaning this up a little bit, we have: $Y_p = \frac{e^{2x}}{3} \int e^x dx - \frac{e^{-x}}{3} \int e^{4x} dx$

When solving this, we use u-substitution on the last integral, and after pulling the terms together we get: $Y_p = \frac{1}{4}e^{3x}$

So, now that we have y_c and Y_p, we can move on to step three, and form the general solution to our problem. $y(x) = c_1e^{2x} + c_2e^{-x} + \frac{1}{4}e^{3x}$

This would be the general solution to the original non-homogeneous differential equation having used the method of variation of parameters.

The last chapter is dedicated to solving chemistry-related problems using differential equations. Here we'll look more closely at the method of how to solve linear first order equations.

8 Modeling with first order linear differential equations, a chemistry problem

In chemistry we have that the rate of a reaction is affected by the concentration or pressure of the reactants. In this example, however, we're going to look at how the concentration affects the problem.

The rate-law or rate-equation is a mathematical description of the relationship between the rate of the reaction and the concentration of the reactants.

Example 8.1. We have a pond that contains 10 million liters of fresh water. Then water containing an unwanted chemical flows into the pond at a rate of 5 million liters per year. The mixed flows out of the pond at the same rate. The incoming chemical has a concentration $\gamma(t)$ that varies with time, periodically, according to the expression $\gamma(t) = 2 + 2\sin(2t)g/L$. Construct a model of the inflow/outflow process and find the amount of chemical in the pond at ant time t. Next, plot the solution.

Notice that we have water flowing in and out at the same times, so the amount of water in the pond stays constant at 10^7 liters. Time, denoted t, is measured in years, and the chemical will be $Q(t)$, measured in grams.

$\frac{dQ}{dt} = rate\,in–rate\,out$

Here $rate\,in$ and $rate\,out$ refer to the rates, or velocity, which the water containing the chemical enters and leaves the pond. Rate in is gives by:

$rate\,in = (5 * 10^6)L/year(2 + \sin(2t))g/liter$

The concentration of the chemical in the pond is $\frac{Q(t)}{10^7}$, so the outflow rate is:

$rate\,out = (5 * 10^6)L/year\frac{Q(t)}{10^7}g/L = \frac{Q(t)}{2}g/year$

Having calculated these, we get the differential equation:

$\frac{dQ}{dt} = (5 * 10^6)(2 + \sin(2t)) - \frac{Q(t)}{2}$,

each term has the units of $g/year$.

From the text we know that there were originally no chemicals in the pond, so we have the initial condition $q(0) = 0$.

Before we move on with the calculations, it would be convenient to make the coefficients a bit more manageable by introducing a new variable defined by $q(t) = \frac{Q(t)}{10^6}$. Now $q(t)$ is measured in millions of grams, or tons. If we substitute this variable into the previous equation, we see that all terms will contain a factor of 10^6, which means it can be canceled. Doing this, we need to transpose the term involving $q(t)$ into the life-hand side of the equation and then we get:

$\frac{dq}{dt} + \frac{1}{2}q = 10 + 5\sin(2t)$

Although the right-hand side is a function of time, q is a constant, so we have that this equations is linear. The next thing we need to do then will be to find the integrating factor: $\mu(t) = e^{\int[P(t)]dt}$.

We have $P(t) = \frac{1}{2}$. Which then gives us the integrating factor: $e^{\int t/2dt} = e^{t/2}$

Now we multiply each term of the equation with the integrating factor. $\frac{dq}{dt}e^{t/2} + \frac{1}{2}qe^{t/2} = 10e^{t/2} + 5\sin(2t)e^{t/2}$

Rearranging the left-hand side, we get: $\frac{d}{dt}e^{t/2}q = 10e^{t/2} + 5\sin(2t)e^{t/2}$

Now we take the integral on both sides and integrate: $\int[\frac{d}{dt}e^{t/2}q]dt = \int[10e^{t/2} + 5\sin(2t)e^{t/2}]dt$

$e^{t/2}q = 20e^{t/2} - \frac{40}{17}\cos(2t)e^{t/2} + \frac{10}{17}\sin(2t)e^{t/2} + C$

Now we divide each term by $e^{t/2}$, simplify and the we have the general solution for $q(t)$. $q(t) = 20 - \frac{40}{17}\cos(2t) + \frac{10}{17}\sin(2t) - Ce^{-t/2}$

If we go back to the initial condition, we can solve the general solution for C to obtain the particular solution. $q(0) = 20 - \frac{40}{17}\cos(0) + \frac{10}{17}\sin(0) - Ce^0$

This gives us $C = -\frac{300}{17}$. So the solution to the initial value problem is: $q(t) = 20 - \frac{40}{17}\cos(2t) + \frac{10}{17}\sin(2t) - \frac{300}{17}e^{-t/2}$

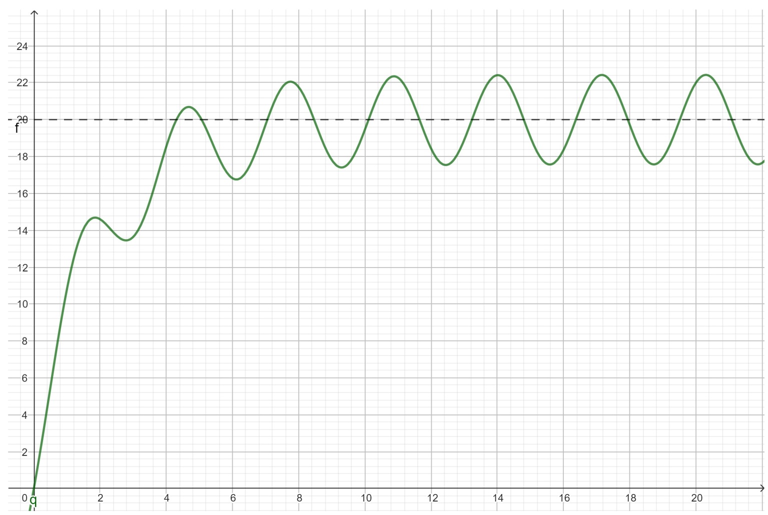

Figure 2:

A plot of the solution is shown in figure 6.1. The figure also show a dotted line along $q = 20$. We can see that the exponential term is significant for small t, but as t increases the significance diminishes. The solution later consists of an oscillation about $q = 20$, due to the sine- and cosine-terms. This tells us that as the years go, the concentration of chemicals in the pond will vary within the value of $q = 20 \pm 2$.

Lastly we'll look at a more extensive example. This example will concern some of the same aspects as the previous example. Here we will also have to use the same inflow/outflow principle.

We have a problem that goes as follows: A tank contains $100L$ of water and $50dkg$ of salt. Water containing a salt concentration of $\frac{1}{4}(1 + \frac{1}{2}\sin(t))dkg/L$ flows into the tank at a rate of $2L/min$. The mixture is well stirred and leaves the tank at the same rate. Find the amount of salt in the tank at any time. The long-term behavior of the solution is an oscillation about a certain constant level. What is this level? What is the amplitude of the oscillation? In this problem we're going to let $Q(t)$ be the amount of salt dissolved in the tank at any time t. The liquid entering the tank will have a different concentration that the liquid leaving the tank.

So, we have a tank that contains a certain concentration of a solution, and we have liquid entering the tank with a different concentration. The two concentrations mixes and then the new solution is pumped out of the tank. Since this is our case, we can say that:

$$\frac{dQ}{dt} = rate \quad in{-}rate \quad out \tag{13}$$

where $\frac{dQ}{dt}$ is the rate the which $Q(t)$ is changing in the tank. *Ratein* is the rate at which $Q(t)$ is entering the tank, and *rateout* is the rate at which $Q(t)$ is leaving the tank. The first thing we need to do to solve this problem is to find the *rate in* and the *rate out*. To find these we need to multiply the concentration times the rate.

$$Rate \quad in = (\frac{1}{4}(1 + \frac{1}{2} + sint)\, d\,\text{kg/L})(2L/min) = \frac{1}{2} + \frac{1}{4}\sin(t)\, d\,\text{kg/min}$$

$$Rate \quad out = (\frac{Q(t)}{100}\, d\,\text{kg/L})(2L/min) = \frac{Q(t)}{50}\, d\,\text{kg/min}$$

In both of the equations above we can see that the units of liters simplify out. So, our differential equation is:

$$\frac{dQ}{dt} = \frac{1}{2} + \frac{1}{4}\sin(t)\, d\,\text{kg/min} - \frac{Q(t)}{50}\, d\,\text{kg/min} \tag{14}$$

If we rearrange equation (7), we can see that it is in fact a linear first order differential equation. Which we can solve by using an integrating factor.

$$\frac{dQ}{dt} + \frac{1}{50}Q(t) = \frac{1}{4}\sin(t) + \frac{1}{2} \tag{15}$$

To solve a linear first order differential equation we first need to put in standard form: $\frac{dy}{dt} + P(t)y = f(t)$. Second, we find the integrating factor: $\mu(t) = e^{\int [P(t)]dt}$. Third, we multiply each term by the integrating factor. Fourth, we find that the left-hand side is the derivative of the product of $\mu(t)$ and y. Fifth, we integrate both sides.

In our case we have $P(t) = \frac{1}{50}$. Which then gives us the integrating factor:

$$e^{\int t/50dt} = e^{t/50} \tag{16}$$

Now we multiply each term by the integrating factor (9):

$$e^{t/50}\frac{dQ}{dt} + \frac{e^{t/50}}{50}Q(t) = \frac{e^{t/50}}{4}\sin(t) + \frac{e^{t/50}}{2} \tag{17}$$

Rewrite the left-hand side as a result of differentiating a product:

$$\frac{d}{dt}e^{t/50}Q(t) = \frac{e^{t/50}}{4}\sin(t) + \frac{e^{t/50}}{2} \tag{18}$$

Take the integral on both sides:

$$\int [\frac{d}{dt}e^{t/50}Q(t)]dt = \int [\frac{e^{t/50}}{4}\sin(t) + \frac{e^{t/50}}{2}]dt \tag{19}$$

Integrating both sides we get:

$$e^{t/50}Q(t) = \frac{25}{5002}e^{t/50}(\sin(t) - 50\cos(t)) + 25e^{t/50} + C \tag{20}$$

Now we divide each term by $e^{t/50}$ and simplify.

$$Q(t) = \frac{25\sin(t)}{5002} - \frac{625\cos(t)}{2501} + 25 + Ce^{-t/50} \tag{21}$$

This is our general solution. Next, we need to use the initial condition mentioned in the problem to solve for C and get a particular solution. We've been told that the tank contains 100 liters of water and 50 dkg of salt, which gives IC: $Q(0) = \frac{1}{2}\, d\,\mathrm{kg/L}$.

Using the IC, we can set $Q = \frac{1}{2}$ and $t = 0$, which cancel out the sin-term and gives us:

$$\frac{1}{2} = -\frac{625\cos(0)}{2501} + 25 + Ce^{0/50} \tag{22}$$

Rearranging the equation we find that the IC requires that $C = \frac{63.150}{2501}$, so our particular solution is:

$$Q(t) = \frac{25\sin(t)}{5002} - \frac{625\cos(t)}{2501} + 25 + \frac{63.150}{2501}e^{-t/50} \tag{23}$$

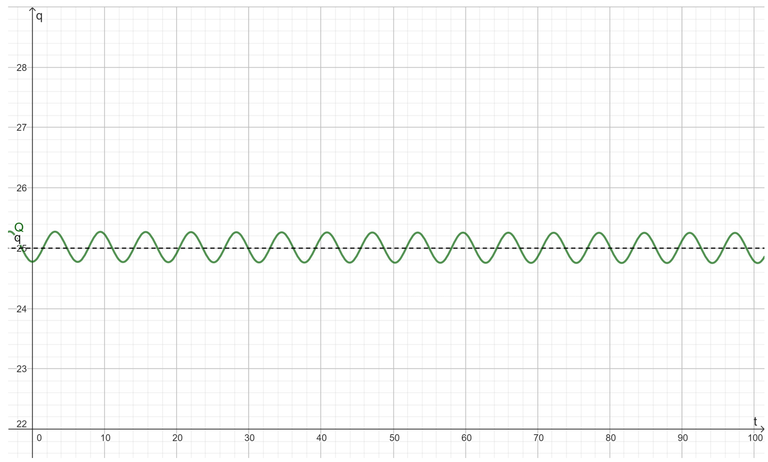

Figure 3:

If we now plot the solution (16) we get a graph that is centred around the dotted line $q = 25$ shown in black in figure 5.1. Considering the fact that $t = time$, the figure doesn't show the negative numbers for t. We see that the solution consists of an oscillation due to the $\sin(t)$ and $\cos(t)$ terms, about the constant level $q = 25$. The amplitude of the oscillation we calculate by taking the term $\frac{625}{2501} - \frac{25}{5002}$, which gives us *amplitude* $\cong 0.249$.

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