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Investigating the Evolution of the COVID-19 Pandemic in Germany Using Physics-Informed Neural Networks

Bachelor Thesis in Computer Science

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Started: May 1, 2024

Finished: September 14, 2024

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Jena, den 14. September 2024

Phillip Rothenbeck

Überblick

German version of the abstract.

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Abstract

English version of the abstract.

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

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1.1 Related work 2

Chapter 2

Theoretical Background 12

This chapter introduces the theoretical knowledge that forms the foundation of the work presented in this thesis. In Section 2.1 and Section 2.2, we talk about differential equations and the underlying theory. In these Sections both the explanations and the approach are strongly based on the book on analysis by Rudin [Rud07] and the book about ordinary differential equations by Tenenbaum and Pollard [TP85]. Subsequently, we employ this knowledge to examine various pandemic models in Section 2.3. Finally, we address the topic of neural networks with a focus on the multi-layer perceptron in Section 2.4 and physics informed neural networks in Section 2.5.

2.1 Mathematical Modelling using Functions 1

To model a physical problem using mathematical tools, it is necessary to define a set of fundamental numbers or quantities upon which the subsequent calculations will be based. These sets may represent, for instance, a specific time interval or a distance. The term *domain* describes these fundamental sets of numbers or quantities [Rud07]. A *variable* is a changing entity living in a certain domain. In this thesis, we will focus on domains of real numbers in \mathbb{R} .

The mapping between variables enables the modeling of the process and depicts the semantics. We use functions in order to facilitate this mapping. Let $A, B \subset \mathbb{R}$ be to subsets of the real numbers, then we define a function as the mapping

$$f : A \rightarrow B. \tag{2.1}$$

In other words, the function f maps elements $x \in A$ to values $f(x) \in B$. A is the *domain* of f , while B is the *codomain* of f . Functions are capable of representing the state of a system as a value based on an input value from their domain. One

illustrative example is a function that maps a time point to the distance covered since a starting point. In this case, time serves as the domain, while the distance is the codomain.

2.2 Basics of Differential Equations 1

Often, the change of a system is more interesting than its current state. Functions are able to give us the latter, but only passively give information about the change of a system. The objective is to determine an effective method for calculating the change of a function across its domain. Let f be a function and $[a, b] \subset \mathbb{R}$ an interval of real numbers, the expression

$$m = \frac{f(b) - f(a)}{a - b} \quad (2.2)$$

gives the average rate of change. While the average rate of change is useful in many cases, the momentary rate of change is more accurate. To calculate this, we need to narrow down, the interval to an infinitesimal. For each $x \in [a, b]$ we calculate

$$\frac{df}{dx} = \lim_{t \rightarrow x} \frac{f(t) - f(x)}{t - x}, \quad (2.3)$$

if it exists. $\frac{df}{dx}$ is the *derivative*, or *differential equation*, it returns the momentary rate of change of f for each value x of f 's domain. Repeating this process on $\frac{df}{dx}$ yields $\frac{d^2f}{dx^2}$, which is the function that calculates the rate of change of the rate of change and is called the second order derivative. Iterating this n times results in $\frac{d^n f}{dx^n}$, the derivative of the n 'th order. Another method for obtaining a differential equation is to create it from the semantics of a problem. This method is useful if no basic function exists for a system. Differential equations find application in several areas such as engineering, physics, economics, epidemiology, and beyond.

Here insert definition of differential equations (take from books)

In the context of functions, it is possible to have multiple domains, meaning that function has more than one parameter. To illustrate, consider a function operating in two-dimensional space, wherein each parameter represents one axis or one that, employs with time and locations as inputs. The term *partial differential equations* (*PDE*'s) describes differential equations of such functions, which require a derivative for each of their domains. In contrast, *ordinary differential equations* (*ODE*'s) are the single derivatives for a function having only one domain. In this thesis, we only

need ODE's.

A *system of differential equations* is the name for a set of differential equations. The derivatives in a system of differential equations each have their own codomain, which is part of the problem, while they all share the same domain.

Tenenbaum and Pollard [TP85] provide many examples for ODE's, including the *Motion of a Particle Along a Straight Line*. Further, Newton's second law states that "the rate of change of the momentum of a body (*momentum = mass · velocity*) is proportional to the resultant external force F acted upon it" [TP85]. Let m be the mass of the body in kilograms, v its velocity in meters per second and t the time in seconds. Then, Newton's second law translates mathematically to

$$F = m \frac{dv}{dt}. \quad (2.4)$$

It is evident that the acceleration, $a = \frac{dv}{dt}$, as the rate of change of the velocity is part of the equation. Additionally, the velocity of a body is the derivative of the distance traveled by that body. Based on these findings, we can rewrite the Equation (2.4) to

$$F = ma = m \frac{d^2s}{dt^2}. \quad (2.5)$$

This explanation of differential equations focuses on the aspects deemed crucial for this thesis and is not intended to be a complete explanation of the subject. To gain a better understanding of it, we recommend the books mentioned above [Rud07, TP85]. In the following section we describe the application of these principles in epidemiological models.

2.3 Epidemiological Models 3

Pandemics, like *COVID-19*, which has resulted in a significant number of fatalities. The question arises: How should we fight a pandemic correctly? Also, it is essential to study whether the employed countermeasures efficacious in combating the pandemic. Given the unfavorable public response to measures such as lockdowns, it is imperative to investigate that their efficacy remains commensurate with the costs incurred to those affected. In the event that alternative and novel technologies were in use, such as the mRNA vaccines in the context of COVID-19, it is needful to test

the effect and find the optimal variant. In order to shed light on the aforementioned events we need to develop a method to quantize the pandemic along with its course of progression.

The real world is a highly complex system, which presents a significant challenge attempting to describe it fully in a model. Therefore, the model must reduce the complexity while retaining the essential information. Furthermore, it must address the issue of limited data availability. For instance, during COVID-19 institutions such as the Robert Koch Institute (RKI)¹ were only able to collect data on infections and mortality cases. Consequently, we require a model that employs an abstraction of the real world to illustrate the events and relations that are pivotal to understanding the problem.

2.3.1 SIR Model 2

In 1927, Kermack and McKendrick [KM27] introduced the *SIR Model*, which subsequently became one of the most influential epidemiological models. This model enables the modeling of infections during epidemiological events such as pandemics. The book *Mathematical Models in Biology* [EK05] reiterates the model and serves as the foundation for the following explanation of SIR models.

The SIR model is capable of illustrating diseases, which are transferred through contact or proximity of an individual carrying the illness and a healthy individual. This is possible due to the distinction between infected beings who are carriers of the disease and the part of the population, which is susceptible to infection. In the model, the mentioned groups are capable to change, *e.g.*, healthy individuals becoming infected. The model assumes the size N of the population remains constant throughout the duration of the pandemic. The population N comprises three distinct groups: the *susceptible* group S , the *infectious* group I and the *removed* group R (hence SIR model). Let $\mathcal{T} = [t_0, t_f] \subseteq \mathbb{R}_{\geq 0}$ be the time span of the pandemic, then,

$$S : \mathcal{T} \rightarrow \mathbb{N}, \quad I : \mathcal{T} \rightarrow \mathbb{N}, \quad R : \mathcal{T} \rightarrow \mathbb{N}, \quad (2.6)$$

give the values of S , I and R at a certain point of time $t \in \mathcal{T}$. For S , I , R and N applies:

$$N = S + I + R. \quad (2.7)$$

¹https://www.rki.de/EN/Home/homepage_node.html

The model makes another assumption by stating that recovered people are immune to the illness and infectious individual can not infect them. The individuals in the R group are either recovered or deceased, and thus unable to transmit or carry the disease. As visualized in the Figure 2.1 the individuals may transition between groups

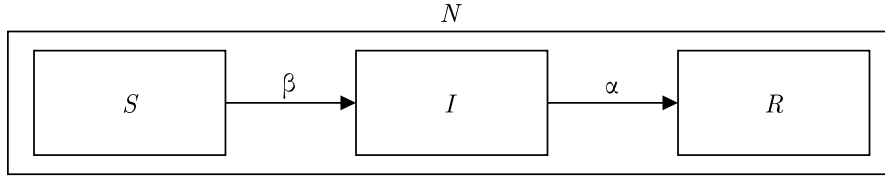


Figure 2.1: A visualization of the SIR model, illustrating N being split in the three groups S , I and R .

based on transition rates. The transmission rate β is responsible for individuals becoming infected, while the rate of removal or recovery rate α (also referred to as δ or ν , *e.g.*, [EK05, MPF23]) moves individuals from I to R .

We can describe this problem mathematically using a system of differential equations (see Section 2.2). Thus, Kermack and McKendrick [KM27] propose the following set of differential equations:

$$\begin{aligned}
 \frac{dS}{dt} &= -\beta SI, \\
 \frac{dI}{dt} &= \beta SI - \alpha I, \\
 \frac{dR}{dt} &= \alpha I.
 \end{aligned}
 \tag{2.8}$$

This, according to Edelstein-Keshet, is based on the following assumption: “The rate of transmission of a microparasitic disease is proportional to the rate of encounter of susceptible and infective individuals modelled by the product (βSI) ” [EK05]. The system shows the change in size of the groups per time unit due to infections, recoveries, and deaths.

The term βSI describes the rate of encounters of susceptible and infected individuals. This term is dependent on the size of S and I , thus Anderson and May [And91] propose a modified model:

$$\begin{aligned}\frac{dS}{dt} &= -\beta \frac{SI}{N}, \\ \frac{dI}{dt} &= \beta \frac{SI}{N} - \alpha I, \\ \frac{dR}{dt} &= \alpha I.\end{aligned}\tag{2.9}$$

In which βSI gets normalized by N , which is more correct in a real world aspect [And91].

The initial phase of a pandemic is characterized by the infection of a small number of individuals, while the majority of the population remains susceptible. The infectious group has not yet infected any individuals thus neither recovery nor mortality is possible. Let $I_0 \in \mathbb{N}$ be the number of infected individuals at the beginning of the disease. Then,

$$\begin{aligned}S(0) &= N - I_0, \\ I(0) &= I_0, \\ R(0) &= 0,\end{aligned}\tag{2.10}$$

describes the initial configuration of a system in which a disease has just emerged.

In the SIR model the temporal occurrence and the height of the peak (or peaks) of the infectious group are of paramount importance for understanding the dynamics of a pandemic. A low peak occurring at a late point in time indicates that the disease is unable to keep pace with the rate of recovery, resulting in its demise before it can exert a significant influence on the population. In contrast, an early and high peak means that the disease is rapidly transmitted through the population, with a significant proportion of individuals having been infected. Figure 2.1 illustrates the impact of modifying either β or α while simulating a pandemic using a model such as Equation (2.9). It is evident that both the transmission rate β and the recovery rate α influence the height and time of the peak of I . When the number of infections exceeds the number of recoveries, the peak of I will occur early and will be high. On the other hand, if recoveries occur at a faster rate than new infections the peak

2.3 Epidemiological Models 3

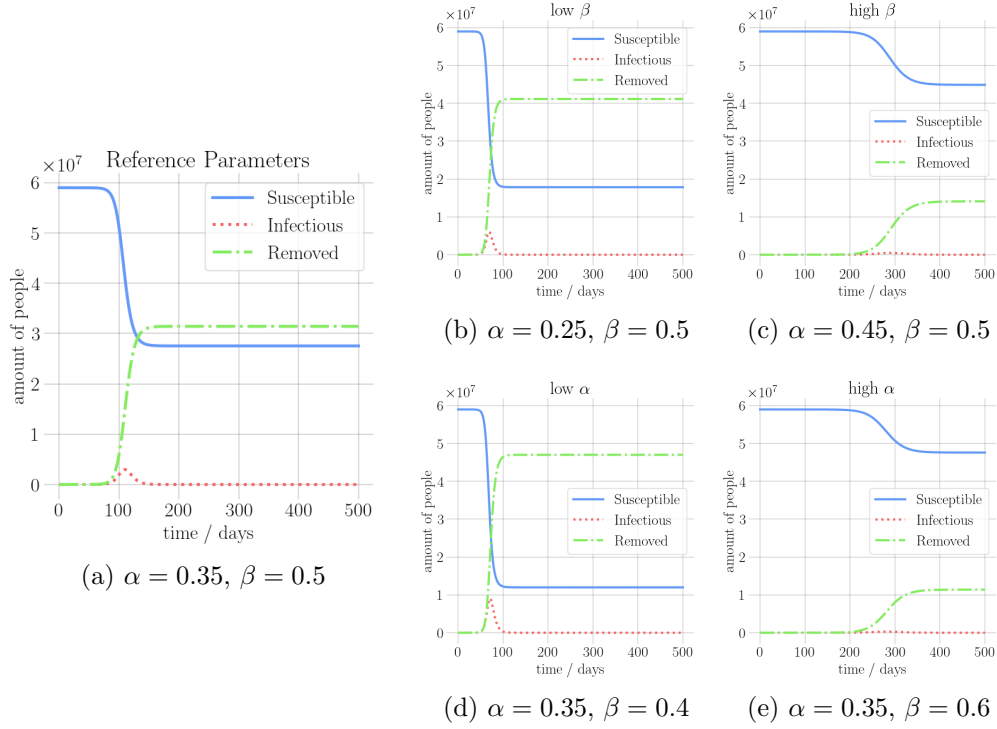


Figure 2.2: Synthetic data, using Equation (2.9) and $N = 7.9 \cdot 10^6$, $I_0 = 10$ with different sets of parameters.

will occur later and will be low. This means, that it is crucial to know both β and α to be able to simulate a pandemic using the SIR model.

The SIR model makes a number of assumptions that are intended to reduce the model's overall complexity while simultaneously increasing its divergence from actual reality. One such assumption is that the size of the population, N , remains constant. This depiction is not an accurate representation of the actual relations observed in the real world, as the size of a population is subject to a number of factors that can contribute to change. The population is increased by the occurrence of births and decreased by the occurrence of deaths. There are different reasons for mortality, including the natural aging process or the development of other diseases. Other examples are the absence of the possibility for individuals to be susceptible again, after having recovered, or the possibility for the transition rates to change due to new variants or the implementation of new countermeasures. We address this latter option in the next Section 2.3.2.

2.3.2 Reduced SIR Model and the Reproduction Number 1

The Section 2.3.1 presents the classical SIR model. The model comprises two parameters β and α , which describe the course of a pandemic over its duration. This is beneficial when examining the overall pandemic; however, in the real world, disease behavior is dynamic, and the values of the parameters β and α change at each time point. The reason for this is due to events such as the implementation of countermeasures that reduce the contact between the infectious and susceptible individuals, the emergence of a new variant of the disease that increases its infectivity or deadliness, or the administration of a vaccination that provides previously susceptible individuals with immunity without ever being infectious. To address this Millevoi *et al.* [MPF23] introduce a model that simultaneously reduces the size of the system of differential equations and solves the problem of time scaling at hand.

First, they alter the definition of β and α to be dependent on the time interval $\mathcal{T} = [t_0, t_f] \subseteq \mathbb{R}_{\geq 0}$,

$$\beta : \mathcal{T} \rightarrow \mathbb{R}_{\geq 0}, \quad \alpha : \mathcal{T} \rightarrow \mathbb{R}_{\geq 0}. \quad (2.11)$$

Another crucial element is $D(t) = \frac{1}{\alpha(t)}$, which represents the initial time span an infected individual requires to recuperate. Subsequently, at the initial time point t_0 , the *reproduction number*,

$$\mathcal{R}_0 = \beta(t_0)D(t_0) = \frac{\beta(t_0)}{\alpha(t_0)}, \quad (2.12)$$

represents the number of susceptible individuals, that one infectious individual infects at the onset of the pandemic. In light of the effects of β and α (see Section 2.3.1), $\mathcal{R}_0 > 1$ indicates that the pandemic is emerging. In this scenario α is relatively low due to the limited number of infections resulting from $I(t_0) \ll S(t_0)$. When $\mathcal{R}_0 < 1$, the disease is spreading rapidly across the population, with an increase in I occurring at a high rate. Nevertheless, \mathcal{R}_0 does not cover the entire time span. For this reason, Millevoi *et al.* [MPF23] introduce \mathcal{R}_t which has the same interpretation as \mathcal{R}_0 , with the exception that \mathcal{R}_t is dependent on time. The definition of the time-dependent reproduction number on the time interval \mathcal{T} with the population size N ,

$$\mathcal{R}_t = \frac{\beta(t)}{\alpha(t)} \cdot \frac{S(t)}{N} \quad (2.13)$$

includes the rates of change for information about the spread of the disease and information of the decrease of the ratio of susceptible individuals in the population. In contrast to β and α , \mathcal{R}_t is not a parameter but a state variable in the model and enabling the following reduction of the SIR model.

Equation (2.7) allows for the calculation of the value of the group R using S and I , with the term $R(t) = N - S(t) - I(t)$. Thus,

$$\begin{aligned}\frac{dS}{dt} &= \alpha(\mathcal{R}_t - 1)I(t), \\ \frac{dI}{dt} &= -\alpha\mathcal{R}_t I(t),\end{aligned}\tag{2.14}$$

is the reduction of Equation (2.8) on the time interval \mathcal{T} using this characteristic and the reproduction number \mathcal{R}_t (see Equation (2.13)). Another issue that Millevoi *et al.* [MPF23] seek to address is the extensive range of values that the SIR groups can assume, spanning from 0 to 10^7 . Accordingly, they initially scale the time interval \mathcal{T} using its borders to calculate the scaled time $t_s = \frac{t-t_0}{t_f-t_0} \in [0, 1]$. Subsequently, they calculate the scaled groups,

$$S_s(t_s) = \frac{S(t)}{C}, \quad I_s(t_s) = \frac{I(t)}{C}, \quad R_s(t_s) = \frac{R(t)}{C},\tag{2.15}$$

using a large constant scaling factor $C \in \mathbb{N}$. Applying this to the variable I , results in,

$$\frac{dI_s}{dt_s} = \alpha(t_f - t_0)(\mathcal{R}_t - 1)I_s(t_s),\tag{2.16}$$

a further reduced version of Equation (2.8) results in a more streamlined and efficient process, as it entails the elimination of a parameter (β) and two state variables (S and R), while adding the state variable \mathcal{R}_t . This is a crucial aspect for the automated resolution of such differential equation systems, as we describe in Section 2.4.

2.4 Multilayer Perceptron 2

In Section 2.2, we demonstrate the significance of differential equations in systems, illustrating how they can be utilized to elucidate the impact of a specific parameter on the system's behavior. In Section 2.3, we show specific applications of differential equations in an epidemiological context. The final objective is to solve these equations. For this problem, there are multiple methods to achieve this goal. On

such method is the *Multilayer Perceptron* (MLP) [HSW89]. In the following section, we provide a brief overview of the structure and training of these *neural networks*. For reference, we use the book *Deep Learning* by Goodfellow *et al.* [GBC16] as a foundation for our explanations.

The objective is to develop an approximation method for any function f^* , which could be a mathematical function or a mapping of an input vector to a class or category. Let \mathbf{x} be the input vector and \mathbf{y} the label, class, or result. Then, $\mathbf{y} = f^*(\mathbf{x})$, is the function to approximate. In the year 1958, Rosenblatt [Ros58] proposed the perceptron modeling the concept of a neuron in a neuroscientific sense. The perceptron takes in the input vector \mathbf{x} performs an operation and produces a scalar result. This model optimizes its parameters θ to be able to calculate $\mathbf{y} = f(\mathbf{x}; \theta)$ as accurately as possible. As Minsky and Papert [MP72] demonstrate, the perceptron is only capable of approximating a specific class of functions. Consequently, there is a necessity for an expansion of the perceptron.

As Goodfellow *et al.* proceed, the solution to this issue is to decompose f into a chain structure of the form,

$$f(\mathbf{x}) = f^{(3)}(f^{(2)}(f^{(1)}(\mathbf{x}))). \quad (2.17)$$

This converts a perceptron, which has only two layers (an input and an output layer), into a multilayer perceptron. Each sub-function, designated as $f^{(i)}$, is represented in the structure of an MLP as a *layer*. A multitude of *Units* (also *neurons*) compose each layer. A neuron performs the same vector-to-scalar calculation as the perceptron does. Subsequently, a nonlinear activation function transforms the scalar output into the activation of the unit. The layers are staggered in the neural network, with each layer being connected to its neighbors, as illustrated in Figure 2.3. The input vector \mathbf{x} is provided to each unit of the first layer $f^{(1)}$, which then gives the results to the units of the second layer $f^{(2)}$, and so forth. The final layer is the *output layer*. The intervening layers, situated between the first and the output layers are the *hidden layers*. The alternating structure of linear and nonlinear calculation enables MLP's to approximate any function. As Hornik *et al.* [HSW89] demonstrate, MLP's are universal approximators.

caption

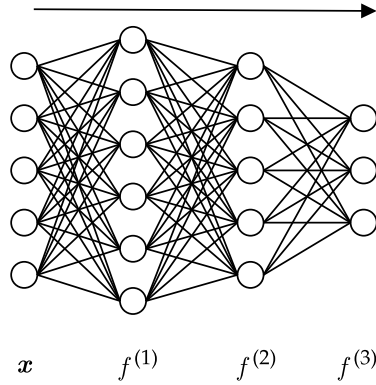


Figure 2.3: A visualization of the SIR model, illustrating N being split in the three groups S , I and R .

The term *training* describes the process of optimizing the parameters θ . In order to undertake training, it is necessary to have a set of *training data*, which is a set of pairs (also called training points) of the input data \mathbf{x} and its corresponding true solution \mathbf{y} of the function f^* . For the training process we must define the *loss function* $\mathcal{L}(\hat{\mathbf{y}}, \mathbf{y})$, using the model prediction $\hat{\mathbf{y}}$ and the true value \mathbf{y} , which will act as a metric for evaluating the extent to which the model deviates from the correct answer. One of the most common loss function is the *mean square error* (MSE) loss function. Let N be the number of points in the set of training data. Then,

$$\mathcal{L}_{MSE}(\hat{\mathbf{y}}, \mathbf{y}) = \frac{1}{N} \sum_{i=1}^N \|\hat{\mathbf{y}}^{(i)} - \mathbf{y}^{(i)}\|^2, \quad (2.18)$$

calculates the squared difference between each model prediction and true value of a training and takes the mean across the whole training data.

In the context of neural networks, *forward propagation* describes the process of information flowing through the network from the input layer to the output layer, resulting in a scalar loss. Ultimately, the objective is to utilize this information to optimize the parameters, in order to minimize the loss. One of the most fundamental optimization strategy is *gradient descent*. In this process, the derivatives are employed to identify the location of local or global minima within a function. Given that a positive gradient signifies ascent and a negative gradient indicates descent, we must move the variable by a constant *learning rate* (step size) in the opposite

direction to that of the gradient. The calculation of the derivatives in respect to the parameters is a complex task, since our functions is a composition of many functions (one for each layer). We can address this issue taking advantage of Equation (2.17) and employing the chain rule of calculus. Let $\hat{\mathbf{y}} = f(w; \theta)$ be the model prediction with $w = f^{(2)}(z; \theta_2)$ and $z = f^{(1)}(\mathbf{x}; \theta_1)$. \mathbf{x} is the input vector and $\theta_1, \theta_2 \subset \theta$. Then,

$$\nabla_{\theta_1} \mathcal{L}(\hat{\mathbf{y}}, \mathbf{y}) = \frac{d\mathcal{L}}{d\hat{\mathbf{y}}} \frac{d\hat{\mathbf{y}}}{df^{(2)}} \frac{df^{(2)}}{df^{(1)}} \nabla_{\theta_1} f^{(1)}, \quad (2.19)$$

is the gradient of $\mathcal{L}(\hat{\mathbf{y}}, \mathbf{y})$ in respect of the parameters θ_1 . The name of this method in the context of neural networks is *back propagation*.

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In practical applications, an optimizer often accomplishes the optimization task by executing gradient descent in the background. Furthermore, modifying the learning rate during training can be advantageous. For instance, making larger steps at the beginning and minor adjustments at the end. Therefore, schedulers are implementations algorithms that employ diverse learning rate alteration strategies.

This section provides an overview of basic concepts of neural networks. For a deeper understanding, we direct the reader to the book *Deep Learning* by Goodfellow *et al.* [GBC16]. The next section will demonstrate the application of neural networks in approximating solutions to differential systems.

2.5 Physics Informed Neural Networks 5

In Section 2.4, we describe the structure and training of MLP's, which are recognized tools for approximating any kind of function. This section, we show that this capability can be applied to create a solver for ODE's and PDE's as Legaris *et al.* [LLF97] describe in their paper. In this method, the model learns to approximate a function using the given data points and employs knowledge that is available about the problem such as a system of differential system. The physics-informed neural network (PINN) learns system of differential equations during training, as it tries to optimize its output to fit the equations.

In contrast to standard MLP's PINN's have a modified Loss term. Ultimately, the loss includes the above-mentioned prior knowledge to the problem. While still containing the loss term, that seeks to minimize the distance between the model

predictions and the solutions, which is the observation loss $\mathcal{L}_{obs}(\hat{\mathbf{y}}, \mathbf{y}) = \mathcal{L}_{MSE}(\hat{\mathbf{y}}, \mathbf{y})$, a PINN adds a term that includes the residuals of the differential equations, which is the physics loss $\mathcal{L}_{physics}(\mathbf{x}, \hat{\mathbf{y}})$ of the PINN and tries to optimize the prediction to fit the differential equations.

2.5.1 Disease Informed Neural Networks 2

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