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

Bachelor Thesis in Computer Science

submitted by

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Jena, den 14. September 2024

Phillip Rothenbeck

40 pages in total

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Überblick

German version of the abstract.

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Abstract

English version of the abstract.

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Chapter 1

Introduction

1.1 Related work

Chapter 2

Theoretical Background

This chapter introduces the theoretical knowledge that forms the foundation of the work presented in this thesis. In Sections 2.1 and 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 multilayer perceptron in Section 2.4 and physics informed neural networks in Section 2.5.

2.1 Mathematical Modelling using Functions

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

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.

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

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

In 1927, Kermack and McKendrick [KM27] introduced the *SIR Model*, which subsequently became one of the most influential epidemiological models. 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, by healthy individuals becoming infected. In the real world 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. To omit this factor of complexity, the model assumes the size N of the population remains constant throughout the duration of the epidemic. The population N is

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

comprised of three distinct groups: the *susceptible* group S , the *infectious* group I and the *removed* group R (hence SIR Model). For S , I , R and N applies:

$$N = S + I + R. \quad (2.6)$$

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

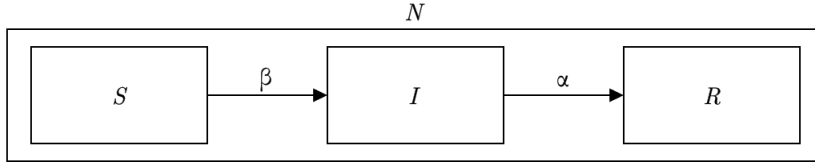


Figure 2.1: SIR Model

based on 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 in the literature) moves individuals from I to R .

In order to model the problem mathematically using a system of differential equations as we describe in Section 2.2, it is necessary to make an assumption serving as the foundation for the model. In their book, Edelstein-Keshet makes 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]. Kermack and McKendrick [KM27] thus propose the following set of differential equations:

$$\begin{aligned} \frac{dS}{dt} &= -\beta SI, \\ \frac{dI}{dt} &= \beta SI - \alpha I, \\ \frac{dR}{dt} &= \alpha I. \end{aligned} \quad (2.7)$$

The system shows the change of 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:

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

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

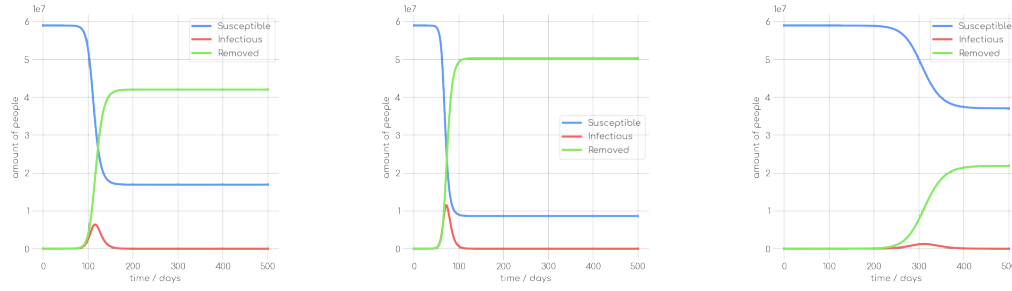
The initial phase of a pandemic is characterized by the infection of a small number of individuals, while the majority of the population remains susceptible. The infectious group has not yet infected any individuals thus neither recovery nor mortality is possible. Let $I_0 \in \mathbb{N}_{\geq 0}$ be the number of infected individuals at the beginning of the disease. Then,

$$\begin{aligned}S(0) &= N - I_0, \\ I(0) &= I_0, \\ R(0) &= 0,\end{aligned}\tag{2.9}$$

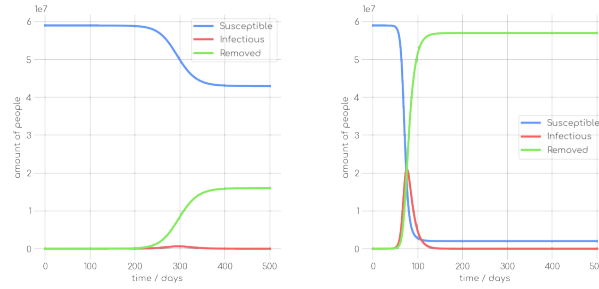
describes the initial configuration of a system in which a disease has just emerged.

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 the pace with the rate of recovery, resulting in its demise before it can exert a significant influence on the population. In contrast, an early, 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 2.8. It is evident that both the transmission rate β and the recovery rate α influence the height and time of occurrence 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

2.4 Multilayer Perceptron



(a) Basic configuration, $\alpha = 0.35, \beta = 0.2$ (b) High α configuration, $\alpha = 0.45, \beta = 0.2$ (c) Low α configuration, $\alpha = 0.25, \beta = 0.2$



(d) High β configuration, $\alpha = 0.35, \beta = 0.3$ (e) Low β configuration, $\alpha = 0.35, \beta = 0.1$

Figure 2.2: Synthetic data, using the Equations 2.8 and $N = 7.9 \cdot 10^6$, $I_0 = 10$ with different sets of parameters.

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

2.3.2 reduced SIR Model

2.4 Multilayer Perceptron

2.5 Physics Informed Neural Networks

2.5.1 Disease Informed Neural Networks

Chapter 3

Methods

3.1 Data Preprocessing

3.1.1 RKI Data

3.1.2 Recovery Queue

3.2 PINN for the SIR Model

3.3 PINN for the reduced SIR Model

Chapter 4

Experiments

4.1 SIR Model

4.1.1 Setup

4.1.2 Results

4.2 Reduced SIR Model

4.2.1 Setup

4.2.2 Results

Chapter 5

Conclusions

5.1 Further Work

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