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Empirical Approach on Uncertainty Analysis of Differential Equations in Mathematical Modeling

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Abstract **Original Research Article**

Uncertainty theory, introduced by Professor Baoding Liu of Tsinghua University in China in 2007, has lately made significant progress. It serves as an advanced and adaptable mathematical tool for modeling uncertainties and handling unforeseen outcomes that may arise when using likelihood and/or fuzzy set approaches, which are sometimes favored alternatively. Mathematical models are used in several academic disciplines to provide accurate quantitative estimations based on facts. Crucially, these mathematical frameworks must offer a dependable evaluation of the certainty in their predictions. Uncertainty quantification (UQ) is a discipline that focuses on delivering accurate and dependable assessments of trust regarding forecasts made by models. Empirical models utilize data and statistical methods to build connections between parameters in a system, whereas mechanistic frameworks are built upon prior knowledge and understanding of the underlying mechanism that governs changes in the overall structure. This article will demonstrate the effectiveness of a data-driven empirical technique in solving ordinary differential equations under conditions of uncertainty. The research aims to determine the practicality and accuracy of its approach compared to existing numerical methods, which may often yield unsatisfactory results.

Keywords: uncertain differential equation, uncertainty quantification, empirical approach, empirical solution, ordinary differential equation uncertainty.

1. INTRODUCTION

Uncertainty theory, introduced by Professor Baoding Liu of Tsinghua University in China in 2007, is a recently developed discipline of axiomatic mathematics that has gained significant popularity. It is primarily utilised to handle the concept of "belief degree" as defined by Liu (2007). Probability is a commonly used theory to model uncertainty and understand random events. However, it may not be enough to address uncertainties related to personal beliefs of individuals (Liu, 2010a).

In order to meet this requirement, uncertainty theory has recently undergone significant development. It functions as a sophisticated and flexible mathematical instrument for representing uncertainties and resolving unexpected results that may occur when employing probability and/or fuzzy set assumptions, which are occasionally preferred alternatives.

Mathematical models are utilised throughout various fields of study to offer precise quantitative data-driven estimations. Significantly, these mathematical algorithms must provide a reliable assessment of the certainty in their forecasts. The discipline of uncertainty quantification (UQ) specializes on generating and presenting precise levels of confidence in forecasts from models. (Shuttleworth *et al.*, 2024).

Empirical models rely on data and statistical procedures to establish relationships between parameters in a system, while mechanistic frameworks are based on previous experience and comprehension of the fundamental process that drives changes in the overall structure (Mas, 2021). In this article, we're going to present the efficacy of data-driven empirical approach in finding the solution when it is worked under uncertainty conditions of ordinary differential equation. The research attempts to establish its feasibility and accuracy over the traditional numerical methods that in certain instances fail to give the desires results.

2. BACKGROUND STUDY

The application of uncertainty theory, which Liu (2007) and Liu (2009) refined, has been fruitful in numerous disciplines, including science, technology, finance, the environment, and more. One early use was ambiguity statistics, which Liu (2010) defined as a set of mathematical techniques for data gathering, analysis, and interpretation based on uncertainty theory. One facet of uncertain analytics is the uncertain assumption test, which uses the idea of uncertainty to determine if a hypothesis is reliable or not based on the data that has been collected. Ye and Liu initiated the present study in 2022. Uncertainty in time series appraisal, uncertain regression modeling, and other areas of uncertain statistics have all adopted the uncertain hypothesis analysis (Ye & Liu, 2023).

Uncertain differential equation (Liu 2008) is employed as a mathematical tool to represent the temporal changes of a dynamic system, adding to the realm of uncertain statistics. Financing (Liu 2013), chemical processes (Tang and Yang 2021), electrical systems (Liu 2021a), drug kinetics (Liu and Yang 2021), software dependability as worked by Liu and Kang in 2022, COVID-19 study by Lio and Liu (2021), holdings issues of Alibaba examined by Liu and Liu (2022), and many more areas have made significant use of uncertain differential equations. In practical applications of unresolved differential equations, the initial step involves estimating the unknown parameters within the equation. The goal of this estimate, which makes use of uncertainty theory, is to fit the data that was collected as precisely as feasible.

Yao and Liu (2020) initially introduced the moment value approximation using the variability analysis method of uncertain differential equation. Afterwards, least squares estimation was studied by Sheng team (2020), minimal compensate estimation was offered by Yang and colleagues in 2020, and the greatest likelihood estimation was proposed by Liu and Liu (2022). But the previously suggested difference-based parameter estimation methods for indeterminate differential equations fail miserably when the measurement intervals are too long. To solve this problem and find a connection between uncertain differential equations and observable data, Liu and Liu (2022) proposed the idea of residuals. They also proposed a novel approach for estimating parameters in uncertain differential equations, utilising the concept of residuals (Ye & Liu, 2023).

When modeling biochemical and biological functions, ordinary differential equations (ODEs) are commonly used. When dealing with beginning circumstances and parameters, ordinary differential equations (ODE) models often face large amounts of ambiguity and unpredictability. Efficient and reliable methodologies for analysing the effects of uncertainty and variability on the dynamical behaviour are particularly crucial, especially when dealing with nonlinear ODEs. An analysis of model sensitivity involves examining how changes in the input variables impact the behaviour of the model, namely its output (Weiße *et al.*, 2010).

In most cases, numerical approaches are used to solve the difficulty. These approaches may include estimating the functional link between the input and output, solving the ordinary differential equation (ODE) for an extensive collection of values to be entered that are produced arbitrarily or quasi-randomly, or determined local sensitivity indices, which are the identified portion of the derivative of the desired result with respect to the input variables. When uncertainty can be reduced to minor disturbances, it is frequently satisfactory to examine its impacts in a localised manner. However, it is challenging to identify in advance whether the uncertainty is small. Additionally, in numerous biological applications, the assumption of minor perturbations is either problematic (e.g., in pharmacokinetics) or has been proven to be incorrect.

The decreasing expenses for sensors, storage facilities, and computational elements resources in the past decade has enabled data-driven exploration methods. Such techniques have had an immense effect on the sciences and mathematical applications by facilitating various innovations in characterising high-dimensional data obtained from experiments (Rudy *et al.*, 2017). From a purely empirical perspective, which is generally a data-driven process, model uncertainty is a concern because estimates may depend on the specific model being used. Hence, the integration of various models to mitigate the variability of models is highly recommended.

Advancements in the numerical solution of ODEs have made it feasible to devise efficient methods that calculate approximate solutions. These solutions are easier for practitioners to read and comprehend, particularly those seeking precise and dependable representations of their mathematical models (Enright, 2012).

Using this methodology, the specialist initially determines the mechanisms that dictate the behaviour of the studied system. Subsequently, leveraging domain-specific expertise on the identified processes, the specialist proceeds to meticulously document a suitable arrangement of the model equations. In contrast to the theoretical approach, the empirical technique relies on gathering and evaluating data via trial and error. The expert selects a class of structures (linear or polynomial, for example) that they believe will work, then adjusts the established parameters of the selected structure and tests the data used for the model adaptation. Iteratively searching for a good model is done if the match isn't close enough. When building models, very little, if any, of the existing domain-specific information is actually use (Todorovski & Džeroski, 2006).

3. RELATED WORKS

This section discusses on the uncertainty conditions and data-driven empirical approaches that are currently being applied and measured in the researches and real life conditions. Considering the research's criteria, ordinary differential equation is given primary focus as the working model and thereafter, the articles are chosen where data-driven approaches are used under uncertainty to obtain feasible values and consequently the model performance measures are described.

For determining the variables in uncertain differential equations, Yao & Liu (2020) utilized a system of moments for the starting time as a means of estimation. Using the one-of-a-kind form of an uncertain differential equation, it was demonstrated that the relationship of the input information adhered to a typical normal uncertainty distribution. These equations were derived by the researchers by replacing the empirical moments of the parameter functions and the observed data with the usual regular uncertain distribution moments. The estimated parameters were given by the answers to these equations. To illustrate the suggested approach of moments, examples were given in both numerically and analytic forms.

Jonckheere (2021) attempted to establish a unified method for estimating differential equations from data that included hidden variables. They conducted a data-driven regression analysis using Lasso-type estimation on the temporal derivative of the variables. The mechanism was evaluated by employing a compendium of functions. These functions included lower-order temporal derivatives of the observable variables. The objective of the study was to create a model capable of quantifying the significance of best-fit data that could differentiate the result accuracy from that when the data contained significant noise.

Extensive numerical instances were demonstrated in the study to show that the proposed method was capable of successfully recovering valuable descriptions of the dynamical system that originated the data. Even, in those cases where certain variables were not observed. Furthermore, due to its reliance on solving a convex optimization challenge, the proposed method was significantly faster than contemporary approaches that lacked in addressing combinatorial issues. Lastly, the model was validated with an actual dataset consisting of temperature time series.

Kuehn (2021) examined how uncertainty in variables in the system was created under a possible significant nonlinear dynamical system and affect the system's bifurcation behaviour. Their model was proposed to calculate the probability of various types of bifurcations (sub-critical versus super-critical) along a particular bifurcation curve. In order to achieve this significant advancement, three methods were proposed: an analytical approach, which involved calculating the probability explicitly using Mellin transformation and inversion; a semi-analytical approach that combined the analytical method with a moment-based numerical value assumption procedure; and a specific sampling-based approach that utilised unscented modification. The model was worked with numerical methods to ensure the extent to which it can be used in uncertainty conditions.

Tang & Li (2021) utilized uncertain differential equations to analyze the individual dynamics of interest rates and stock prices over time. The researchers utilized the method of moments to estimate the variables in uncertain differential equation according to empirical observations. They utilized the provided interest rate and stock models to determine the value of European options and then analyze how these values compare to real-world observations. Ultimately, the stochastic financial model presented a conundrum.

Lejarza & Baldea (2022) presented a machine learning framework to distinguish the compatible equations in the form of ordinary differential equations when worked in noisy experimental data sets. In order to derive simple governing equations from an enormous number of basis functions, their suggested approach evaluated successive subsets of measurement data and used statistical deduction. The proposed system used a state-of-the-art numerical discretization approach to reduce estimation mistakes caused by gradient estimating something. Researchers sought for ways to enhance the model by making it more resilient to noise and stiffer overall. The approach was able to effectively identify simple ruling principles in nonlinear dynamical systems, even when there was a lot of measurement noise. In fact, it performed better than the most advanced frameworks currently available in the literature.

The multi-fidelity Monte Carlo (MFMC) method was developed by Du and Su (2022) to examine the variability of nonlinear partial differential equations. It makes use of data-driven low-fidelity approaches. In the beginning, the nonlinear PDEs were transformed into ODEs via the use of finite discretising difference or the Fourier adjustment. In order to generate effective nonlinear low-fidelity models for the ODEs system, the shortened dimension model and the discrete empirical interpolation method (DEIM) were employed.

To provide the best estimate of the statistics, the MFMC method was used to combine the high-fidelity and low-fidelity model outputs. Results from experiments with the nonlinear Schrodinger and Burgers' equations show that the MFMC method, which is based on a data-driven low-fidelity model, outperforms the traditional Monte Carlo method in terms of computational simplicity.

Noorani & Mehrdoust (2022) proposed an innovative approach to estimate uncertain parameters of a stock model influenced by the Liu process. Parameter estimation was split into two parts by the suggested method. Part one was to use the information at hand to create an optimized artificial neural network, and part two was to use that network to estimate the unreliable variables in the model. In order to optimize the artificial neural network and resolve the parameter guessing issue, because the Nelder-Mead algorithm was employed. The main benefit of the approach being described is that it may be used to forecast future data without worrying about how the estimate difficulty is impacted by the intervals amongst observations. Demonstrating a comparison methodology reveals the potential effectiveness of the suggested strategy for non-linear issues, in which artificial neural network topologies exhibit strong performance.

The study by Zhou *et al.,* (2023) identified seven well characterized subfields related to mathematical uncertainties, that is, uncertainty in the axiomatic framework, in developing, in sets, in logic, in differential equations, in analysis of risks, and in relationships are all subfields of uncertainty.The domains with the most papers are those dealing with uncertain calculations, including differential equations and computing. Furthermore, we develop indices of maturity and current focus based on variables like citations, total documents, volume of highly referenced literature, and half-life to evaluate the research potential of sub-fields.

As indicated by these metrics, uncertain procedures have garnered significant attention in recent years due to their high potential for advancement. The principal areas of investigation in this study are uncertain linear quadratic optimization, the best supervision of discrete-time unresolved processes, and equivocal an extra period reward procedures. In addition, ambiguous risk analysis, which analyzes predicted deficits, risk related to investments, and the structural dependability of platforms with built-in uncertainty, is ranked second among risk analysis techniques.

4. CONCEPTUALIZATION AND METHODOLOGY

The research is conceptualized to provide the evidence of fundamental potency of empirical approach that can be utilized in finding the solution of ordinary differential equation (ODEs)when they are solved under uncertain conditions. The underlying approach aims to reduce the chances of false effort and provide the best-fit route to achieve accuracy and fastness in obtaining the desired solution when they are used in the said conditions.

Furthermore, the practical usability of empirical approach in solving the ODEs in uncertainty condition at real time scenario is particularly explored and analysed. For that a latest real life condition is examined where ODE model is used to estimate a result by applying the data-driven empirical approach. Thereafter, the significance of using empirical model is justified. Overall, the study focuses the core objectivity of revealing the feasibility of empirical method over the other contemporary models, such as computational and probabilistic models so that the technique can be fully utilized to work out with advance technology, such as, machine learning or neural net platforms.

The study can also be extended to ensure the role of empirical approach for differential equations of dynamic form and operational methodologies that can ideally exclude noise and provide the desired results with good accuracy score.

5. FINDINGS AND DISCUSSION

Here, we present two different scenario, (i) one based on model-based approach of finding solution of ordinary differential equations (ODEs) in uncertainty condition; and (ii) the other where ODE model is used to estimate a real time condition added with uncertainty. In both the case, data-driven empirical approach is used and the model performance is evaluated accordingly.

i. Solution of Ordinary differential equations (ODEs) in a Two-Stage Indirect Approach to Estimate the Derivatives of the State

Model Details:

The two-stage approach, as outlined by Bradley and Boukouvala (2021), addresses two distinct issues associated with regression in order to take into account the variable parameters of the mechanistic model. In the preliminary stage, the variables comprising the data-driven framework are modified based on the first findings of the measurements. During the second phase, the settings of the logical ODE are determined utilizing the state and derivative estimations of the data-driven model. This is achieved through the initial resolution of the ensuing regression issue.

$$\text{Min} \sum(x_{k,j,mess} - x_{k,j,pred})^2 + \lambda\sum w^2 \text{ ------------------- (1)}$$

$$\text{s.t.}\frac{dxk}{dt} = \text{NN}(x_k, w) \text{ ------------------------------------- (2)}$$

At this point we integrate a NODE with respect to the standalone variable t in order to determine and forecast the state factors x_k at time points j, where j runs from 1 to J, while k extends from 1 to K. With the help of a term for regularizing and the total number of squared deviations between the forecasts made by the model and what was found in the facts, the objective function was minimized by adjusting the parameter values of the neural network.

Performance Discussion:

A regularizing penalty element is added to the goal function and compounded by a hyperparameter λ in order to take into consideration the several parameters in the neural network. Incorporating the learnt NODE from the beginning of the data set at time t0=0 to the end at time tf yields derivative projections once the NODE (Neural Ordinary Differential Equation) has been trained.

Using the same procedure parameters as the observed data. The NODE models derived products using state projections at times when measurable data is available. Inequalities 3 and 4 reflect the second part of the two-stage method, which entails developing a nonlinear program (NLP) in order to discover the components of the original mechanical ordinary differential equation (ODE).

This study compares the efficiency of algebraic data-driven models—specifically, algebraic neural networks—with that of more conventional computational methods for predicting system derivatives, and it finds that the latter are superior. This system is also used to demonstrate the ability of the indirect method to estimate parameters for mechanical ordinary differential equations (ODEs) with very nonlinear components.

A study of contrasts was done involving the computational needs of the NODE2 condition methodology and the standard direct strategy in order to evaluate its efficacy. The findings of this study were summarized after it was run on without noise training data. A preset amount of 10 undetectable nodes was put in a neural network situated in the node for this experiment.

When discussing the direct method, "compute time" is how long it takes to train the components of the mechanical ordinary differential equation (ODE). Stage 1 of the indirect technique's computing time consists of fitting the neural ODE settings, and stage 2 is solving the NLP for the mechanistic parameters.

The time comparison does not account for the hyperparameter modification. In a nutshell, the time required to handle a single NODE is already included in stage 1. Although the NODE 2-stage approach's computing expenditure will grow due to hyperparameter modification, the grid search cross-validation technique may be parallelized to reduce this computation time.

The work also made a significant contribution by demonstrating how to train neural Ordinary Differential Equations (ODEs) using integration. To determine the dynamics of a system, the standard two-stage approaches use algebraic data-driven models. Because directly integrating differential equations is computationally costly, this is done instead. Using NODEs for derivative estimations, the suggested method successfully brings integration back into the two-stage approach, even if it is only present in the first phase.

The time required to train algebraic data-driven models, like the one used in this study, is far lower than that required to learn neural ordinary differential equations (ODEs). Stage 2's natural language processing (NLP) issue cannot be solved using their derivative estimates, nevertheless. Neuronal Ordinary Differential Equations (ODEs) are able to record data on derivatives effectively, according to this study's reasoning. This supports the use of NODEs regardless of the additional computing expense resulting from integration and gradient evaluation during conditioning.

Contrarily, training neural ODEs takes more time than a conventional artificial neural network (NN), but it's still faster than directly estimating the settings of the underlying mechanism. The study's neural network architecture was smaller than typical deep learning schemes, but there were many more elements to fit to the NODE than to the mechanistic version.

The accuracy was significantly enhanced when NODEs were used as the interpolating model. System derivatives could be computed using other data-driven models. Unfortunately, this study did not have the time or resources to conduct a thorough comparison with all methods. Because splines and other algebraic interpolating frameworks fail to take the required derivatives into consideration, we expect NODEs to perform better.

There are computational benefits to using the neural ODE-based approach rather than directly integrating mechanical ODEs. But the best part is that it can find the mechanical parameters with little to no scaling and no prior knowledge of their values. Mechanistic differential equations involving the parameterization of very nonlinear operators, such logarithmic functions and the exponential form, show the most gain in measurement of parameters.

ii. Use of Ordinary differential equation (ODE) based model to estimate the time variant infection and reporting rate in COVID-19 pandemic time

Model Details:

The project, known as Steuerungs-Prognose von Intensiv medizinischen COVID-19 Kapazitäten (SPoCK), utilizes various data sources and use data-driven methods to predict the number of occupied ICU beds. The scope of the project is shown in the figure below as discussed in the scholarly article of (Refisch *et al.*, 2022):

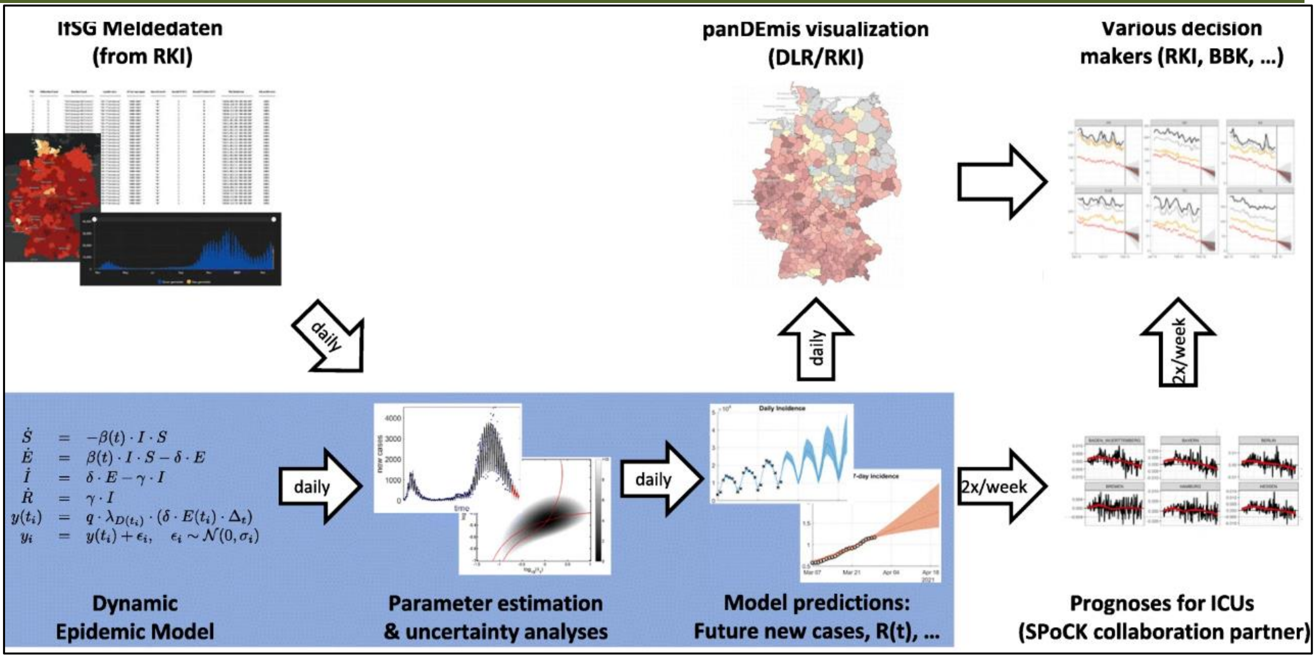

Figure 1: Schematic Diagram Showing the SPoCK program forecasts the requisite hospital capacity of Intensive Care Units (ICUs) for patients with COVID-19. An important variable that must be forecasted is the quantity of latest reported cases from the RKI, which is shown by the blue box. The findings are used for graphically demonstrate DLR logic and management members, such as the BBK, RKI, and local and regional health authorities. (*Source: Refisch et al., (2022)*)

Compartmental models or Susceptible-Infected-Recovered (SIR)-like models are commonly used in this research to describe the spread of infectious diseases. Typically, both methods involve dividing the population into subgroups that have distinct characteristics. Entities are able to shift between specific populations with the help of transitioning rates, which, along with the starting values of those subpopulations, define the system's evolution through time. The validated Susceptible-Exposed-Infected-Recovered (SEIR) model provides the ordinary differential equation (ODE) characterization of the compartment wise-segmented scheme that is given below.

$$
\begin{aligned}
\dot{S} &= -\beta(t)\cdot I\cdot S/N \\
\dot{E} &= \beta(t)\cdot I\cdot S/N - \delta\cdot E \\
\dot{I} &= \delta\cdot E - \gamma\cdot I \\
\dot{R} &= \gamma\cdot I
\end{aligned}
$$

The variable N represents the entire population, and it is equal to the sum of the variables S, E, I, and R. To display time derivatives, one uses the dot format. Also, ο, γ, and δ stand for the rates of distribution, infectiousness, and mortality or treatment, correspondingly. The reason for selecting this model class is its conciseness, which is crucial for frequent evaluation, and its ability to accommodate a more adaptable infection time compared to the usual SIR model.

Performance Discussion:

Multiple research have addressed the issue of time-dependent infection rates in various ways. During the initial stages of the COVID-19 global mass health hazard, researchers analyzed the effects of various non-pharmacological interventions (NPIs) using step functions that implemented β(t) using several versions of smoothed step functions. The goal was to determine how various NPIs fared. These strategies are sometimes only applicable to certain time periods when the infection frequency is expected to be constant or consistently decreasing or increasing. However, we want to use a more holistic approach that permits the infection rate to fluctuate freely within the given timeframe, meaning it can drop or rise more than once.

It is essential to have an accurate description of the COVID-19 transmission dynamics because it is affected by numerous elements that can change during the continuing COVID-19 pandemics.

- Multiple Non-Pharmaceutical Interventions (NPIs) are implemented, revoked, and reintroduced in an iterative manner.
- The sample member's adherence to regulatory measures fluctuates throughout time.
- Seasonal factors, such as meteorological conditions, result in variations in the likelihood of infection.
- Mutations modify the physiological mechanisms that underlie disease transmission and other related issues.
- Vaccinations decrease the proportion of the population that is susceptible.
- Air pollution can exacerbate the severity of COVID-19.

Typically, there are multiple model categories and architectures that can be used to represent the same event. The differences in the mechanical architecture of different frames make it generally hard to transfer approximation values across them. To tackle this issue, we avoid using any prior knowledge about parameter values in the optimization process and instead depend only on data.

There are just three fixed factors that are established in advance, which are the initial numbers of individuals in the affected, revealed and regained states:S_{init}, E_{init}, and R_{init}. The time point zero (t_0) is defined as the earliest day with a minimum of 100 reported cases, in order to uphold the premise of well-mixing in ODE modelling. S_{init} represents the entire population of the specific region, as reported by the Federal Statistical Office of Germany.

In order to measure the level of uncertainty in the model's predictions, our forecasting tool offers confidence intervals in addition to the suggested predictions. In this case, we talk about two main sources of doubt: uncertainty about parameters and uncertainty about approaches. As explained in the Profile likelihood analysis portion, the first approach is to simulate every prospective attribute arrangements that match the data that has been collected. As explained in the part called "Averaging of approaches," the second method includes doing the investigation using a lot of different models.

To predict variables using data, numerous kinds of methods can be used, such as ordinary differential equation (ODE) models or stochastic differential equation (SDE) models, regardless of the mixed results. Employing a System Dynamics Engineering (SDE) method could prove advantageous in tiny locations characterized by minimal infection rates or during periods of exceptionally low overall infection figures.

In such instances, the spread of infection is mostly driven by local outbreaks, and the population is not thoroughly mixed, making the use of ordinary differential equations (ODEs) inefficient. In a well-mixed system, the infection probability for all susceptible individuals is uniformly distributed, and the spread of infection is governed by an average infection probability. The premises that were used to make the ODE approach for the selected geographical units make sense, and the model was changed in a good way. Our main goal was to create an effective approach that lets us analyze data every day and make precise projections.

6. CONCLUSION

As discussed in the above two cases, both models showed the improved accuracy of data-driven empirical approach when it is applied on the ODE model under uncertainty condition. The first approach as shown is worked on experimental machine learning based model that used data-driven interpolation as a better solution approach that traditional direct conventional algebraic approach. Although, the model exhibited a few data oriented limitation.

In the second model, the ODE is utilized in estimating the real time patient count estimation that is worked in data-driven approach and the data are evaluated in terms of their noise content. Here too, the data-driven stochastic approach showed accurate determination of result under uncertainty condition over the tradition computational methods. Thus, we can say that empirical approach has its own efficacy under uncertainty condition to tackle time variant data sources and provide the result.

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