Informed Deep Learning for Epidemics Forecasting

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Abstract. The SARS-CoV-2 pandemic has galvanized the interest of the scientific community toward methodologies apt at predicting the trend of the epidemiological curve, namely, the daily number of infected individuals in the population. One of the critical issues, is providing reliable predictions based on interventions enacted by policy-makers, which is of crucial relevance to assess their effectiveness. In this paper, we provide a novel data-driven application incorporating sub-symbolic knowledge to forecast the spreading of an epidemic depending on a set of interventions. More specifically, we focus on the embedding of classical epidemiological approaches, i.e., compartmental models, into Deep Learning models, to enhance the learning process and provide higher predictive accuracy.

Keywords. Machine Learning, Deep Learning, Universal Differential Equations, Compartmental Models

1. Introduction

The 21st century has been marked by an ever-increasing level of human activity on the planet, favoring a global interconnection and new development opportunities. Unfortunately, this phenomenon has led to environment-invasive operations that altered the equilibrium of our ecosystem, paving the way for the emergence of novel zoonotic viruses [1]. Among these, *airborne* diseases are the most worrying, due to their capability of spreading at a fast pace (e.g, SARS, MERS, H1N1). Most notably, the recent outbreak of Sars-CoV-2 [2], which started in late 2019, in Wuhan, China. This unexpected scenario has brought to light the unpreparedness of policy-makers and the consequent lack of prompt and effective responses apt at containing the spread of the virus and mitigating its effects on global health and socio-economic systems.

For this reason, the creation of preemptive mechanisms and the assessment of the impact of countermeasures on the evolution of the epidemic is of crucial relevance to help policy-makers in the development of effective containment plans. Such mechanisms should be capable of coping with the complexity and uncertainty aspects ingrained in the epidemic phenomena, which are hard to solve with traditional approaches from the statistical and epidemiological fields - analytically expressing the relationship between virus spreading, countermeasures, and socio-economic impacts is a non-trivial task. In this sense Artificial Intelligence can bring great benefits; for instance, the recent advances made in the field of Deep Learning (DL) [3] allow to extract useful insight from data and

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correctly forecast future scenarios, whereas Combinatorial Optimization [4] can exploit such insights to produced informed decisions [5].

In this paper, we provide two data-driven approaches incorporating sub-symbolic knowledge to forecast the spreading of an epidemic w.r.t. a set of interventions aimed at counteracting its effects. Thus, the main objective is to identify a model mapping a set of interventions onto the epidemiological curve representing the number of infected individuals in the population. More precisely, we consider **N**on-**P**harmaceutical-**I**nterventions (NPIs), namely policies that address the epidemic from an administrative perspective (e.g., lockdowns, public transport access, schools openings) rather than a medical or clinical ones [6,5].

These models can be then used to produced effective policies to battle an outbreak - for example they could be used to boost Combinatorial processes returning an intervention plan to contain the spreading of the disease.

The main contributions of this paper are:

- Two methodologies forecasting the trend of an epidemic based on a set of interventions
- The integration of traditional epidemiological techniques in DL models
- An approach to fit the parametrization of a dynamic system based on temporal data

The rest of the paper is structured as follows: Section 2 provides the basis to understand the methodologies proposed in the paper, as well as relevant work related; in Section 3, we will present the two methodologies at the core of this paper; in Section 4, we will showcase the experimental results on our frameworks; finally, in Section 5, we will close the paper with some final comments and pointers to future improvements.

2. Background

The problem of capturing and predicting the dynamics of epidemics is a well-known and widely studied problem. There have been many attempts to model these phenomena in the past, from mathematical models to complex networks, and, more recently, agent-based methods and machine learning [7,8]. Our work is mainly concerned with the use of classical mathematical approaches to enhance the learning process. In this section, we will introduce such methods, as well as, prior work related to our research.

2.1. Mathematical Models

Mathematical models are among the first and most successful methods used to approximate the spreading of a virus during an epidemic. One of the most widely known and effective mathematical models in epidemiology are *Compartmental Models* [9]. This class of methods partitions the population into compartments, or categories, describing the status of subgroups of individuals w.r.t. the disease. The flow of people from one state to the other is described by a set of parametrized Ordinary Differential Equations (ODE). Compartmental methods can be classified into two broad categories:

- **Deterministic**, that given a certain initial state of the compartments and a set of parameters, can fully determine the final state of the model through the transition formulas

- **Stochastic**, which are probabilistic formulations of Compartmental models where uncertainty is represented through stochastic processes, such as Markov Chains and the Monte Carlo method. The behavior of the system can only be observed through a simulation

An intuitive example of deterministic compartmental models, is the SIR model, which divides the population into **S**usceptible-**I**nfected-**R**ecovered, in which the transition to one category to the other is described by the following differential system:

$$\frac{dS}{dt} = -\beta \, \frac{S \cdot I}{N} \tag{1}$$

$$\frac{dI}{dt} = \beta \, \frac{S \cdot I}{N} - \gamma I \tag{2}$$

$$\frac{dS}{dt} = \gamma I \tag{3}$$

, where β is the *infection rate* — defined as the *average number of contacts* per person for each time step, multiplied by the *probability of disease transmission* in a contact between a susceptible and an infectious subject — and γ is the *recovery rate* — defined as the inverse of the *recovery period*; N is total amount of the population.

Compartmental models are the backbone of epidemics forecasting, as they provide a clear understanding of the mechanisms underlying the disease spreading allowing for a deeper theoretical analysis of the phenomenon. However, these methods do not provide a fine-grained approximation of an epidemic. For instance, Compartmental models assume a homogeneous and well-mixed population with full connection, i.e., all individuals make contact at every time step, failing to represent the individual human behavior which is characterized by high variance and heterogeneity. Moreover, these models do not allow to assess the impact of a restrictive measure enacted to contain the spreading of a virus, limiting their usability in decision scenarios.

To address these issues many are the variants of the basic SIR model, such as: **SEIR**, or **S**usceptible-**E**xposed-**I**nfected-**R**ecovered, and the **SIRD**, **S**usceptible-**I**nfected-**R**ecovered-**D**eceased. More recently, **SIDARTHE** [10] which extends the number of compartments and interaction among them to better represent the COVID-19 virus.

2.2. Related Work

In this section, we briefly introduce some of the main research work focused on forecasting the spreading of a virus through Deep Learning.

Deep Learning. A straightforward approach to approximate the dynamics of an outbreak is two use classical DL techniques designed to handle temporal series. The literature presents a plethora of successful applications ranging from simple Recursive Neural Networks (RNN) to more sophisticated applications involving Long-Short Term Neural Networks (LSTM) [11,12]. Other approaches rely, instead, on the use of Convolutional Neural Networks, which allow capturing local trends in the data, namely temporal locality when it comes to temporal series [13].

Epidemics find a natural representation in graph networks. Indeed, among the most im-

portant models approximating these phenomena we find complex network [14]. For this reason, an increasing trend employs Graph Neural Networks (GNNs) to predict the dynamics of an outbreak. In particular, message-passing GNNs, which simulate the contact among individuals in the population, have produced encouraging results [15,16].

Hybrid Deep Learning. The rise of DL in recent years has led to a crossover of different disciplines, giving birth to a variety of hybrid approaches encapsulating different methodologies. Predictive epidemiology has been involved in this process, where classical methods (e.g, mathematical models and complex networks) have been embedded in the learning process of Deep Neural Networks (DNNs). In [17,18], the authors propose a hybrid approach involving Auto-Regressive models, approximating the linear component of the data, and a DNN capturing non-linearity in the epidemic trend.
More recently, we have seen an attempt to encapsulate into learning processes mathematical models, and in particular Compartmental models. The main idea is to approximate the parametrization of the dynamic system through the use of a Feed-Forward Neural Network (FFNN). In [19], this approach is applied to the COVID-19 epidemic in India, where the parameters describing the transitions among the compartments of the model are learned through an incremental learning approach allowing to improve iteratively the DNN without training it on the whole dataset every time is updated; in [20], a similar approach is applied to data relative to the COVID-19 epidemic in South Korea.
Another interesting approach proposes an RNN trained using a data sample augmented through a simulation based on a SEIR model [21] .

Mapping Interventions and Infected. While the previously cited research work deals mostly with modeling the epidemics spread and predicting its evolution, in this work we want to go a step further. Our focus is on the use of Deep Learning to forecast the *impact of containment measures on the epidemiological curve*. To the best of our knowledge, very few attempts involving Machine Learning have been made by the scientific community in this direction. Most notably [5], in which authors have developed an LSTM mapping NPIs into the new daily infected cases of SARS-CoV-2.
Our methods, partially differentiate from this approach by allowing us to predict the values for each of the categories in the Compartmental model used to frame the epidemic.

3. Informed Deep Learning for Epidemics

In this paper, we present two DL-based approaches encapsulating neuro-symbolic knowledge to improve the training process in DNNs. The central idea is to exploit the prior knowledge provided by compartmental models as a mathematical background theory to frame the dynamics of the outbreak. This is achieved by building a deterministic, parametric model of the epidemic based on the differential equations provided by the SIR model, where the parametrization itself is learned as a function of a set of interventions. The final approach provides the means to assess the impact of different containment policies on the underlying compartmental model, i.e., the SIR model.

Formally, we are trying to approximate part of an ODE using a DNN. This method was first proposed with **Universal Differential Equation** (UODE) [22]. The idea of UODE is to approximate part of the dynamic system using a **Universal Approximator**, such as a DNN:

$$u' = f(u,t,U_\theta(u,t))$$

, where u is the state of the mechanistic model, f is the differential equation, t is the current time step, and U_θ is the Universal Approximator, which is trained to optimize a cost function based on the current state of the dynamic system.

The two methods presented in this paper start from the intuition provided by UODE, and try to define two distinct ways to tackle this problem, namely:

- **Interventions Sequential Mapping**: which recovers the parametrization of the SIR model from a historical series, then maps the interventions onto the parameters (Section 3.1)
- **End-to-End Interventions Mapping**: that learns the mapping in an end-to-end fashion (Section 3.2)

3.1. Interventions Sequential Mapping

The Interventions Sequential Mapping (ISM) model aims at approximating the epidemic using two data-driven models enhanced by a SIR model. The first model is a neural network approximating the parametrization of the SIR model based on the historical series representing the epidemiological curve (i.e., the daily number of infected individuals), while the second model, is a regressor - a second DNN - mapping the NPIs onto the SIR parametrization, thus effectively providing a model capable of forecasting the virus spreading depending on a set of containment policies.

In the general formulation, a SIR model requires the definition of the values of β and γ. Both parameterizations are time-dependent since they might vary based on different contextual changes. We can apply a simplification by arguing that γ tends to keep a roughly constant value during an epidemic — since the average recovery period is affected only by clinical and treatment issues — which eventually become stable whenever a practice is established — rather than depending on possibly variable external factors. For instance, many studies point to 14-16 days as the average recovery time for COVID-19 [23,24] On the contrary, β is highly variable, it is influenced by continuously floating variables such as environmental conditions, containment measures, and ultimately people's behavior. Under these assumptions, we can assign a fixed value to γ, which we can infer using historical data, while we express β as a time-dependent variable $\beta(t)$. To recover the β series, the first model is built as a custom neural network composed of: a number of layers equal to the time window covered by the data - with length T - where each layer is composed of a set of neurons representing the state of the SIR model at time i; a series of T weights represent our current belief on the parametrization of the model, i.e. $\beta(t)$.
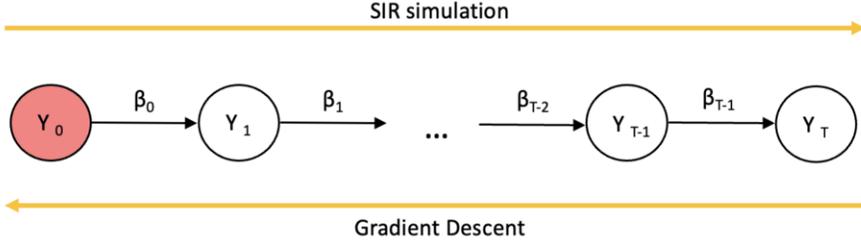
Figure 1. Architecture of the first model used to fit the parametrization of the SIR curve

The forward phase runs the SIR simulation - thus using the belief parametrization - given an initial state, $y_0 = (S_0, I_0, R_0)$. This allows to compute a cost function which will guide the optimization process updating the weights of the network, i.e. our belief β series:

$$Loss(y, \hat{y}) = \frac{1}{T} \sum_{t=0}^{T} (y_t - \hat{y}_t)^2 + \lambda \Omega_\beta$$

, where $y_i = (S_i, I_i, R_i)$ represents our supervision, whereas $\hat{y}_i$ the output of the forward step; Ω_β is a regularization term ensuring there are not steep changes in the β series and λ its weighting coefficient.

The regularization term formally enforces a soft constraint on β. Intuitively, abrupt changes in the values of $\beta(t)$ are unrealistic, therefore the discrepancy between β at time $i-1$ and i is unlikely to be very large. This can be expressed through a penalty term of this form:

$$\Omega_\beta = \frac{1}{T-1} \sum_{t=1}^{T} max(0, \beta_t - \beta_{t-1})$$

We can see that changes in the β series of high magnitude lead to increasing values of the regularization penalizing the loss function. The regularizer is weighted using a λ coefficient which is optimized during the training process using a Lagrangian dual method based on sub-gradient descent [25].

After retrieving the parametrization of the SIR model, we approximate the relation between the NPIs and $\beta(t)$ using a DNN. In this phase, we can add other input variables to help better approximate the mapping NPI-*beta*. For instance, if we are aware of a seasonal behavior of the disease (e.g., flu, COVID-19), adding the average temperature for the time window considered might help better encapsulate the epidemiological trend.

$$\tilde{f}(SIR_t, NPI_t, X_t) = y_{t+1}$$

, where SIR_t and NPI_t represents respectively the state of the SIR curve and the interventions at time t, while X_t exogenous variables concurring to a better approximation of environmental aspects of the epidemic.

Overall, the ISM method represents a valid data-driven solution to approximate the epidemic by exploiting pre-existing knowledge regarding epidemics. However, we will introduce a second model integrating the mechanisms of the Compartmental model into the learning process, allowing for a more refined approximation of the epidemiological curve.

3.2. End-To-End Interventions Mapping

The second approach tries to overcome the use of two distinct models to approximate the relation between NPIs and the epidemic curve. The idea is to create an End-to-End Interventions Mapping (EIM), which encapsulates the compartmental model into the learning process. The peculiarity of this approach is to directly map the NPIs into the epidemiological curve, exploiting the SIR model as a theoretical framework but without striving to explicitly fit the real β parameters. Based on the UODE approach, we can rewrite the SIR transition system, assuming to have a universal approximator - in our case a DNN - for β:

$$\beta_{t+1} = U_\theta(SIR_t, NPI_t, X_t)$$

, where SIR_t is the state of the SIR model at the current time, NPI_t represents the interventions at time t, and X_t exogenous variables concurring to a better approximation of environmental aspects of the epidemic. In this context, the architecture of the model consists of a traditional Feed-Forward neural network where the parametrization, θ, can be optimized via gradient descent based on the following loss function:

$$Loss_\theta(y, \hat{y}) = \frac{1}{N} \sum_{t=0}^{T-1} (y_t(U_\theta(SIR_t, NPI_t, X_t)) - \hat{y}_{t+1})^2$$

, where y_i represents the state of the SIR model at time i, based on the parametrization provided by the universal approximator.

4. Experimental Results

In this section, we present the main experimental results. We decided to test the models on a *synthetic benchmark*, generated starting from a SIR simulation, which allowed us to test the two approaches in an ideal setting. We then proceeded to experiment on a real time series to verify the usability of the frameworks in more practical scenarios.

4.1. Experimental Setup

The experiments were performed on an Azure Virtual Machine with 64 non-multithreaded AMD EPYC 7V12 processor cores, 448 GiB of system memory, and four Nvidia Tesla v100. Each test instance is defined using different initial conditions, i.e., y_0, which allow to generate multiple epidemic scenarios, e.g., different type of disease or different social environments. The models are trained assuming prediction horizons of a week, meaning that the learning target is relative to a week after the state described by input conditions. The architecture of the models across training instances is kept fixed, namely, 4 layers with 16 neurons each, which allows to focus on other parameter-dependent behavior and have a fair comparison among the different approaches.

Baseline Model.   To compare the results of our approaches, we established a *baseline model*, namely a simple regression network mapping the NPIs on the SIR curve. This allows to assess the improvements of the model w.r.t. the naive approach, thus proving that the integration of DNN with compartmental model can improve the learning process.

Evaluation Metrics.   All the models are evaluated with a test set, which is the result of a split on the original dataset holding out 30% of the samples. We then evaluated the performance of each approach using Mean Squared Error, Mean Absolute Error, and Mean Average Percentage Error, as well as the training time for each experimental instance.

4.2. Integration Method

Both models require a numerical iterative method to solve the ODE associated with the transition formula of the Compartmental model. We decided to use the simplest integration technique available, namely the Euler's method. The idea is that given an initial condition, y_0, the state of the dynamic system at time $t + 1$ can be computed as follows:

$$y_t = y_{t-1} + h f(y_{t-1})$$

, where f represents the differential equations associated to a state transition, and h the step size. The step size, a sub-unitarian increment w.r.t. to the time step, is of crucial relevance to determine the accuracy of the overall integration process - in our case, the value h is determined by a hyperparameter K, where $h = \frac{1}{K}$. Indeed, the general rule is that the smaller the increment step the higher the accuracy of the final result, as shown in Figure 2. During the experimental phase, we decided to test the models for increasing values of K, namely 1, 10, and 20.
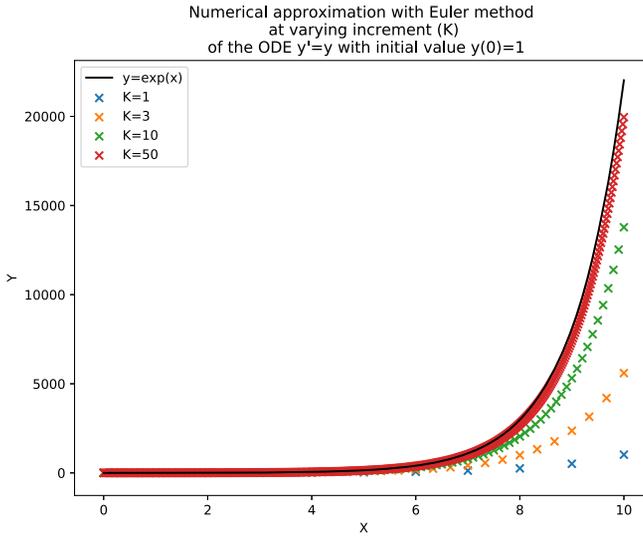
Figure 2. In reference to the example ODE $y' = y$ with initial condition $y(0) = 1$, the graph reports the exact solution $y = e^x$ (black curve) and numerical approximations obtained employing the Euler Method with different increments.

4.3. Synthetic Data

The first round of experiments was held on a set of synthetic data. We decided to proceed with an ideal sample before moving to a real-world application - often the data available are restricted to past epidemics, which do not encapsulate the plethora of possible behavior that might be observed during an outbreak. This allowed to remove some of the confounders present in natural phenomena such as epidemics, e.g., social dynamics, resilience of the population.

Data are created starting from a SIR simulation with a set of the initial condition, S_0, I_0, R_0, γ, and β, which were changed to generate different epidemic curves. The data are relative to 52 weeks, almost a year, in which the outbreak is taking place.

The interventions are generated randomly; to each NPI we associated a *strength*, namely the degree of their impact on the curve, measured with a value between 0 and 1, and an *effect*, that depending on its strength is going to affect the epidemic, i.e., the SIR curve. In Figure 3, we can see an example of a SIR model in time and the perturbation introduced by 5 random NPIs.

4.3.1. Results

The result of the experiments on the synthetic dataset are presented in Table 1, while in Figure 4 we present the reconstruction of the infected curve on the synthetic dataset. As we can observe both models, ISM and EIM, perform better than the baseline model, which does not approximate the curve effectively. Both models confirm that for increasing value of K the performance of the model are more accurate. The ISM approach improves consistently on the Baseline, however the EIM model shows a dramatic decrease in the error, along with lower computation costs.

(a) SIR (b) SIR-NPI
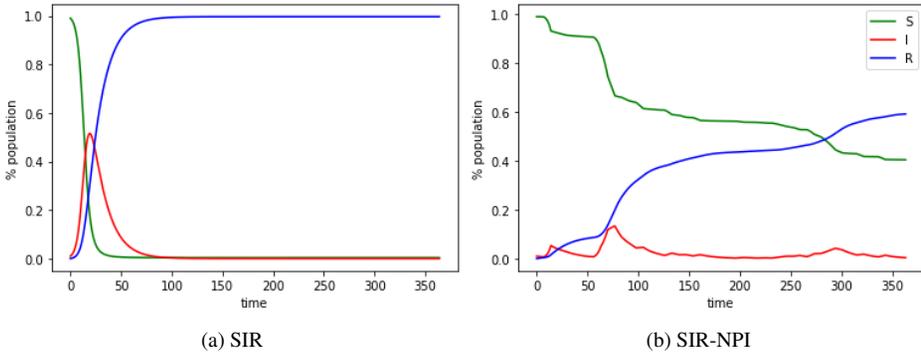
Figure 3. On the left side a SIR curve generated with following initial conditions: $S_0 = 0.99$, $I_0 = 0.01$, $R_0 = 0.0$, $\gamma = \frac{1}{15}$, $\beta = 0.3$. On the right side the same curve computed generating a random set of 5 NPIs for each time step.

(a) Baseline (b) ISM vs. EIM
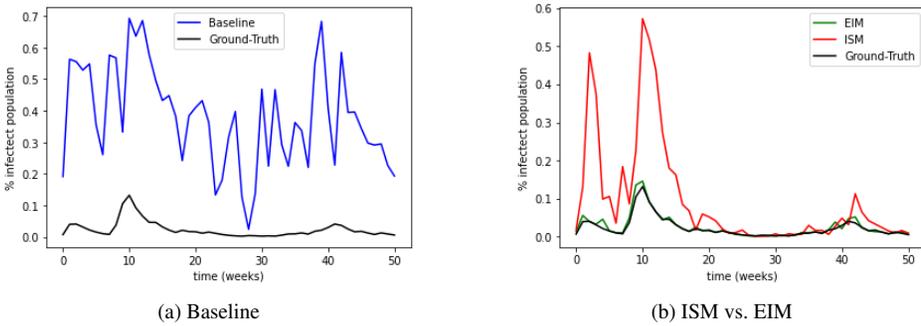
Figure 4. Reconstruction of the infected curve using the Baseline model (left), and the ISM and EIM models (right). The curve in generate with the following initial conditions $S_0 = 0.99$, $I_0 = 0.01$, $R_0 = 0.0$, $\gamma = \frac{1}{15}$, $\beta = 0.3$, and $K = 10$

Model		MSE	MAE	MAPE	Time(ms)
NN		0.0057	0.047	$2,2 \cdot 10^8$	**754**
ISM	K=1	0.0017	0.0089	0.16	321541
	K=10	0.0018	0.0088	0.16	1531902
	K=20	**0.0013**	**0.0086**	**0.14**	2935251
EIM	K=1	0.00027	0.0038	0.08	2199
	K=10	**0.00021**	**0.0035**	**0.09**	7283
	K=20	0.00019	0.0036	0.10	13222

Table 1. Evaluation Baseline (NN), ISM and EIM models on the Synthetic Dataset

4.4. Real-World Data

We extended the experimental results using a real case scenario. In particular, we used the COVID-19 data provided by the Italian "Protezione Civile" (Civil protection), which

monitors the pandemic in Italy from its start[2]. We focused on ICU hospitalization since they are not affected by the floating number of tests performed on the population.

Concerning the interventions, we relied on the public data provided by the Oxford Covid-19 Government Response Tracker, which recorded NPIs relative to economic, political, and health policies enacted to counteract the spreading of SARS-CoV-2 and its effects. Figure 5 displays the SIR curve associated with the pandemic in Italy from February 24th, 2020, to May, 8th, 2022. The plot shows how the infected curve (i.e. red line) has different peaks, representing the multiple waves of the COVID-19 epidemic. Also in this case, the models are trained assuming a time step of a week.

(a) SIR   (b) Infected
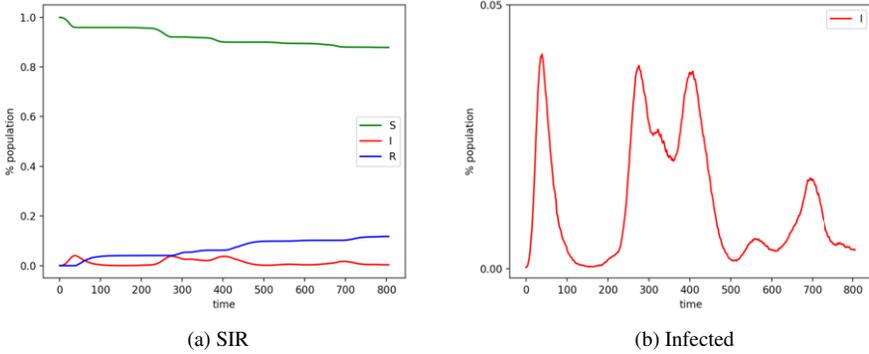
Figure 5. SIR curves of SARS-CoV-2 epidemic in Italy - form February 24th, 2020, to May, 8th, 2022

4.4.1. Results

The results of the experiment are presented in Table 2, while in Figure 6 we present the reconstruction of the curve of ICU hospitalization in Italy. Again, both models show better performances w.r.t. the baseline. In this context, the EIM approach is the most accurate.

(a) Baseline   (b) ISM vs. EIM
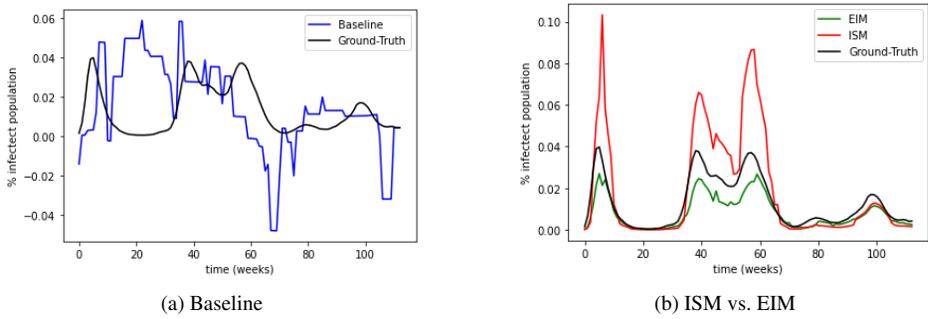
Figure 6. Reconstruction of the curve representing the ICU hospitalization in Italy using the Baseline model (left), and the ISM and EIM models (right), assuming $\gamma = 1/16$ and $K = 10$

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[2]https://github.com/pcm-dpc/COVID-19

Model		MSE	MAE	MAPE	Time(ms)
NN		0.00069	0.016	$1.8 \cdot 10^{12}$	1147
ISM	K=1	0.012	0.058	0.33	661705
	K=10	0.0092	0.048	0.32	3099793
	K=20	0.0090	0.049	0.31	6154240
EIM	K=1	0.000019	0.0026	0.28	2865
	K=10	0.000054	0.0030	0.26	9153
	K=20	0.000015	0.0024	0.23	23236

Table 2. Evaluation Baseline (NN), ISM and EIM models on the Real-World Dataset

5. Discussion

The two methods proposed in this paper proved to be effective for both synthetic and real-world data, approximating accurately a variety of scenarios, including very hard instances such as the outbreak of COVID-19 in Italy. Beyond tackling a classical problem of epidemiology (namely, predicting the spreading of a virus in time) with new techniques, these approaches allow us to assess the effects of policies apt at countering the negative impact of the disease.

Following we highlight some of the crucial aspects associated to the use of these models.

Human Readable Results.   The embedding of Compartmental models into the learning process allow for a better understanding of the dynamics of an outbreak. Indeed, the categories, or compartments, provide us with the tools and language to understand how the disease moves within the population, providing the means to describe mathematically its behavior using the grounding of the real-word data. This is a powerful tool making the results readable to non-experts that need to understand and justify decisions based on these models.

Multiple Application.   Both models are a solution to the same problem, however, their payout is different. The ISM approach, proves to be computationally expensive, however it accurately and explicitly recovers the parameters of the SIR model. This represents a truthful approximation of the actual value of the β series in the training window, which can be useful when the parametrization of the model is of interest. Moreover, this approach can be extended to other dynamic systems. The EIM approach, instead, provides similar results to ISM but with lower computational costs. This model does not provide an accurate parameterization of the compartmental model, however, proves to be effective w.r.t. the learning task.

Decision Support Systems.   The methods proposed in this paper can be used as tools to facilitate a decision-making process during an epidemic. As the COVID-19 pandemic has taught us, rapid responses to novel viruses are of crucial relevance to prevent losses of lives and stem its effect on the economy and, in general, society.
Following the idea proposed in [5], this process can be automated if combined with an optimization process. The idea is to boost the combinatorial problem to find the best policy to contain the disease, using the DL model to shape the relationship between interventions and the epidemic. This can be achieved using: either a **Black-Box approach**, in which the model is used as an heuristic by the solver [26], that is agnostic w.r.t. the

structure of the model, or **embedding the model**, namely codifying the model directly into the combinatorial process. Both methods proposed in this paper would be suitable for such application and we plan to extend this work in such direction.

Future Works.   Ultimately, we want to point out two major improvements to the current state of the work: First, the models we propose are not restricted to the use of a SIR model; one of the models cited in Section 2 might be more suitable depending on the type of virus and the environment in which the outbreak takes place. Additionally, we could assess the performances of the models using different integration methods. As previously stated, we chose the simplest integration method available, which does not exclude the use of more sophisticated approaches, such as Runge-Kutta methods of higher degree.

6. Conclusion

The recent outbreak of COVID-19 has caught policy-makers unprepared. A fast response to this exceptional scenario is of crucial relevance. To this end, quickly assessing the impact of interventions apt at counteracting the spreading of the virus and its negative effect on the social and economical structure is decisive. In this paper, we have proposed two DL-based models capable of forecasting the trend of an epidemic depending on a set of NPIs. Both models incorporate methods from traditional epidemiology to improve the learning process. The results prove our methods to be effective in forecasting the dynamics of an outbreak both in an experimental setting, simulating different environmental conditions, and on real-world data. Future work will be focused on further improving the experimental results through methodological refinements, as well as incorporating the model into automatic decision processes.

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