Accelerating multiagent epidemic modeling with surrogate-based methods

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***Abstract*—In this study, we explore the potential of machine learning models as surrogates for computationally intensive probabilistic models. Traditional multi-agent models (MAM) for forecasting epidemic outbreaks, specifically acute respiratory infections, are accurate but require significant computational resources and time. We propose a surrogate Auto Encoder (AE) to approximate the outputs of these MAMs efficiently. The results indicate that the AE can effectively approximate the MAM outputs, significantly reducing the computation time while maintaining acceptable accuracy. This surrogate model serves as a preliminary assessment tool to decide whether running the full MAM is necessary, thereby saving resources. However, the AE struggles with inheriting the stochasticity of the MAM, resulting in minimal variation in predictions for identical inputs. Despite these limitations, our findings suggest that machine learning surrogates hold promise for accelerating multiagent epidemic modeling, which enhances the applicability of the latter for the epidemic surveillance.**

***Index Terms*—mathematical epidemiology, multiagent modeling, surrogate methods, autoencoders**

I. Introduction

Probabilistic models play a critical role in simulating and understanding the dynamics of epidemic outbreaks. These models, especially multi-agent models (MAMs) [1], are effective in capturing the complex interactions within populations that lead to the spread of diseases. However, the detailed and stochastic nature of these models makes them computationally intensive and time-consuming, limiting their practical usability, especially in scenarios requiring quick decision-making.

To address these challenges, we explore the potential of using machine learning models as surrogates for these traditional probabilistic models. Surrogate models can significantly reduce computation times by approximating the outputs of complex simulations with simpler and faster predictive models. In this study, we focus on employing Auto Encoder (AE) [2] and Variational Autoencoder (VAE) [3] architectures to serve as a surrogate model for a multi-agent model used in forecasting acute respiratory infections.

II. Background and Motivation

Multi-agent models (MAMs) simulate the interactions of agents (individuals) within a population to predict the spread of diseases. While these models are highly accurate and provide detailed insights, their execution can be prohibitively slow. For instance, simulating an epidemic in a large city might take several hours or even days, making it impractical for real-time decision-making.

To overcome this limitation, surrogate models can be used. A surrogate model is a simpler, faster approximation of a complex model. By training a surrogate model on the outputs of the MAM, we can achieve similar results in a fraction of the time [4]. This study investigates the use of an Auto Encoder, a type of generative neural network, as a surrogate for the MAM.

III. Previous work

Surrogate models have been widely used in various domains to approximate complex and computationally expensive models. They serve as efficient alternatives to direct simulations, providing significant speed-ups while maintaining a reasonable level of accuracy. One common application is in the field of engineering design optimization, where surrogate models like Kriging, radial basis functions, and polynomial regression are frequently employed to predict outcomes based on a limited number of expensive simulations [5],[6].

In recent years, the rise of machine learning techniques has further expanded the scope and efficacy of surrogate models. Autoencoders (AEs) and Variational Autoencoders (VAEs) have emerged as powerful tools for dimensionality reduction and generative modeling.

In the context of surrogate modeling for engineering applications, AEs and VAEs have demonstrated substantial potential. For instance, Ling, Kothe & Mullan (2019) [7] used VAEs to develop a surrogate model for predicting the aerodynamic performance of airfoils, achieving a significant reduction in computational cost compared to traditional methods. Similarly, A. Matveeva and V. Leonenko [8] utilized Gaussian process regression (GPR) as a surrogate model to replace detailed simulations of COVID-19 propagation.

These advancements highlight the growing relevance of AEs and VAEs in surrogate modeling, providing a strong foundation for exploring their application in generating test samples for complex systems.

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IV. Methods

A. Data Collection

In this study, we utilized synthetic incidence data for a hypothetical city with a population of 4,000 inhabitants generated by the MAM developed earlier by the authors [10]. This choice was due to the lack of comprehensive data from larger urban centers. The MAM simulated the spread of ARI by varying two key parameters: alpha (transmission rate) ranging from 0.2 to 0.9 in increments of 0.05, and lambda (recovery rate) ranging from 0.5 to 0.9 in increments of 0.1. Each pair of parameters resulted in multiple simulation runs, providing diverse outbreak scenarios and capturing the stochastic nature of the MAM. The training dataset included 201 examples, while the test set comprised 99 examples. Each simulation output was truncated to 50 days to standardize the data.

B. Architecture

An Auto Encoder (AE) is a type of artificial neural network used primarily for unsupervised learning of complex distributions. It consists of two main components: an encoder that compresses the input data into a latent space representation, and a decoder that reconstructs the input data from this latent space. In this study it was initially set to use a Variational Autoencoder (VAE) over a standard AE. The VAE was selected due to its ability to learn a low-dimensional representation of the data while incorporating probabilistic elements. This makes it particularly effective for approximating the outputs of the MAM (Mathematical Model for Disease Prediction), as it provides not just point estimates but also a measure of uncertainty.

The key advantage of using a VAE lies in the incorporation of Kullback-Leibler Divergence (KLD) [9] in the loss function, which regularizes the latent space to follow a prior distribution, typically a Gaussian. This regularization encourages the latent space to be more structured and continuous, which can be beneficial for generating smooth and realistic reconstructions and for downstream tasks that may benefit from such structured latent representations.

C. Training

Despite these theoretical advantages of VAE, practical issues emerged during training. The combined loss function, which included Mean Squared Error (MSE) and KLD, was intended to balance reconstruction quality with regularization of the latent space. However, we encountered significant instability issues with the KLD term (see Fig. 1), especially when using the SiLU activation function.

These instability issues manifested as gradient explosions, where the gradients during backpropagation became excessively large, causing the loss to diverge rather than converge. This problem was exacerbated by the KLD term, which added a complex probabilistic component to the optimization process. As a result, the training process became highly erratic, and the model failed to learn meaningful representations of the data. Despite attempts to mitigate this instability by adjusting hyperparameters and employing gradient clipping, the combination of MSE and KLD loss proved too volatile.

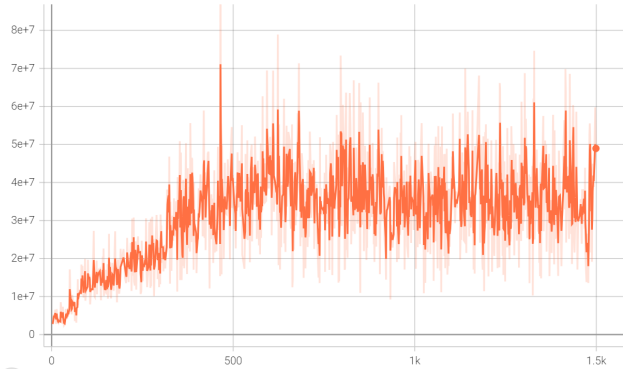

Fig. 1. KL Divergence Loss

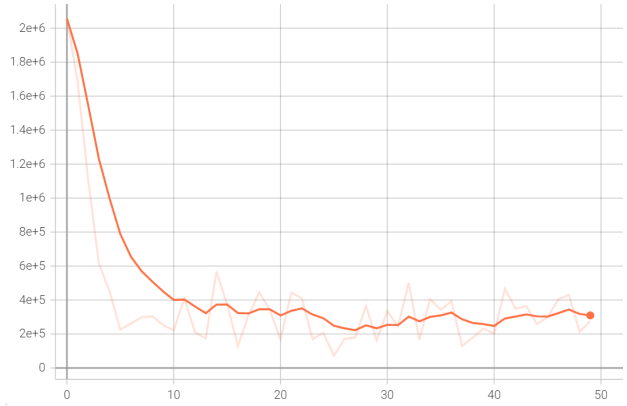

Fig. 2. MSE Loss

Consequently, the decision was made to revert to a standard AE architecture, excluding the KLD term from the loss function. This adjustment simplified the model, focusing solely on minimizing the MSE for reconstruction. While this compromise meant losing the probabilistic benefits of a VAE, it significantly stabilized the training process (see Fig. 2). The AE was able to learn effective latent representations without the numerical issues that plagued the VAE.

Despite this shift, there was a slight compromise in the R^2 metric, indicating a marginal reduction in the model's explanatory power. However, the stability and reliability of the training process with the AE ultimately outweighed the potential benefits of the VAE with KLD. The AE provided a robust framework for predicting disease incidence, achieving consistent and reliable performance across the dataset.

D. Calibration

In Subsection A of this chapter, it was stated that the model employs the parameters α and λ for prediction purposes. However, in real-world scenarios, these parameters are also obscured from us and are more of an abstraction. In situations where predictions are required, we propose the following

solution to address this issue. By analyzing the incidence rates over the first n days, we can infer potential values for alpha and lambda. Subsequently, the top-k potential candidates are averaged, yielding the values that are then fed into the autoencoder.

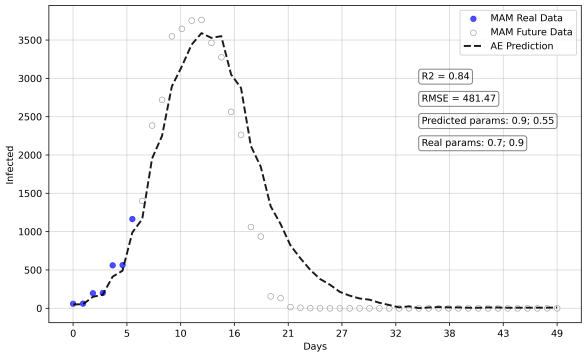

Fig. 3. Prediction example

Moreover, the proposed method is intended to mitigate the inherent uncertainty associated with the hidden nature of these parameters. By leveraging early-stage data to estimate the parameters, we aim to enhance the robustness and accuracy of the predictive model. The approach underscores the importance of parameter estimation in the initial phase, which subsequently informs the autoencoder's input, thereby facilitating more reliable predictions.

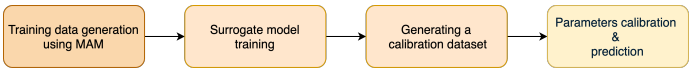

Fig. 4. Full model pipeline

V. Results

The AE demonstrated robust performance on the test set, achieving reliable approximations of the MAM outputs. Considering top-k = 7 and n days = 3 for α, λ calibration and next 43 days reconstruction, we delivered mean of $R^2 = 0.63$, $RMSE = 581$ for sum of 50 days outbreak. Moreover, we achieved peak incidence prediction $accuracy = 0.38$, taking into account the 1-day margin of error. The accuracy of fitting to the known incidence points (calibration error) and the difference between the expected and the actual incidence trajectory (prediction error) are given in Table 1.

The data points depicted in Figure 5 illustrate the prediction bias associated with the peak day (dt) and the ratio of modeled to actual outbreak peak heights (dh). Accurate estimation of the parameters α and λ is essential for the validity of our model. Figure 6 presents the absolute differences between the selected values of α (da) and λ (dl). The optimal scenario is indicated by the intersection of the vertical dashed line (where $dt = 0$) and the horizontal dashed line (where $dh = 1$), signifying accurate peak prediction, as well as the intersection

TABLE I
AE Model metric results

	RMSE	R^2
Calibration		
Min	12.91	-73.72
Mean	127.1	-2.2
Median	112.5	0.81
Max	419.9	0.99
Prediction		
Min	235.8	-1.75
Mean	624.6	0.59
Median	552.88	0.81
Max	1484.4	0.96
Full Timeline		
Mean	**581**	**0.63**

of the vertical dashed line (where $dl = 0$) and the horizontal dashed line (where $da = 0$).

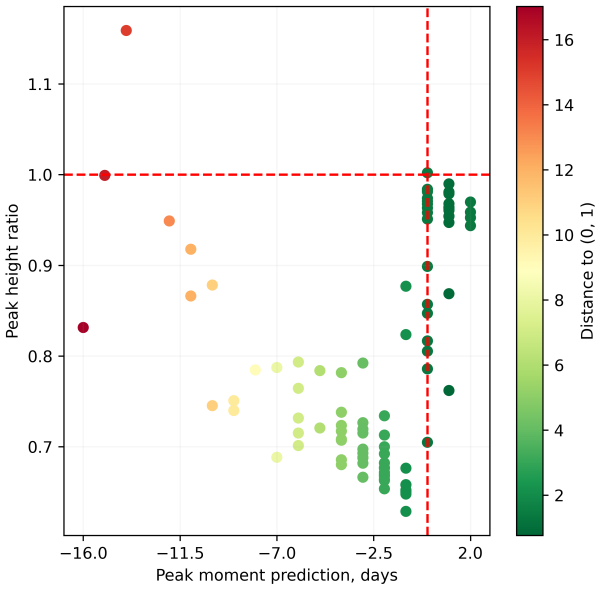

Fig. 5. Biases of the peak and ration prediction.

It is crucial to note that the surrogate model did not replicate the MAM's stochastic nature, resulting in almost identical predictions for given inputs. Despite this, the model's efficiency makes it a valuable tool for preliminary assessments.

To quantify the benefit from the surrogate model in terms of speed-up, compared to the initial MAM, the following calculations were made. Suppose the time taken to generate a sample using the MAM is T_{MAM} and the time taken to generate a sample using the AE model after training is T_{AE}. Let T_{train} be the time required to train the AE model. The

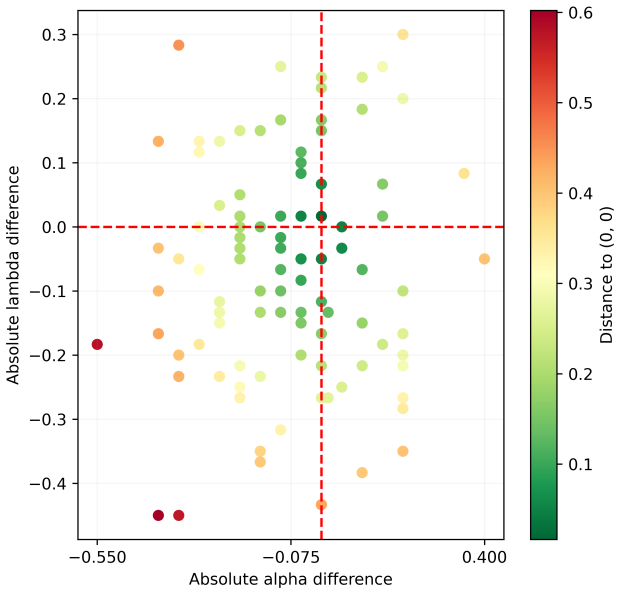

Fig. 6. Biases of the alpha and lambda selection.

TABLE II
TIME CONSUMPTION (MS)

	MAM	AE
Calibration		
Min	–	4.14×10^1
Mean	3.52×10^5	4.50×10^1
Max	–	6.61×10^1
Prediction		
Min	3.16×10^4	4.96×10^{-1}
Mean	6.35×10^4	9.56×10^{-1}
Max	1.02×10^5	6.73×10^1

total time saved S after generating N test samples using the AE/VAE model can be expressed as:

$$S = N \cdot (T_{MAM} - T_{AE}) - T_{train} \tag{1}$$

Assuming data from Table 2, $T_{MAM} = 4.15 \cdot 10^5 ms$, $T_{AE} = 4.6 \cdot 10^1 ms$, $T_{train} = 1.3 \times 10^7 ms$:

$$N = \frac{T_{Train}}{T_{MAM} - T_{AE}} \approx 31.5 \tag{2}$$

Therefore, after predicting approximately 32 samples, the time saved by using the AE model would surpass the time spent on training it. Beyond this point, the AE model offers substantial time savings.

VI. DISCUSSION

The value of this work lies in its ability to speed up the generation of test samples for complex systems by using autoencoders. These models can create high-quality approximations of test samples much quicker than direct simulations by learning a simplified representation of the original data.

It is crucial to consider the time trade-off involved. Training the AE models can be time-consuming, especially when scaling up. Despite this initial time investment, once trained, the models can perform simulations much faster than traditional methods, making them particularly useful in situations requiring a large number of simulation runs over time. Paritularly, this is often the case in epidemic surveillance, when one needs to regularly rerun simulations with updated input data, perform sensitivity analysis and test various "what-if" scenarios in case of cost-effectiveness analysis for disease control measures. Ultimately, the usage of surrogate approaches such as autoencoders, could greatly enhance the attractiveness of multiagent modeling approach for the centers for disease control, which might help perform more elaborative retrospective analysis and forecasting of disease outbreaks.

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