
Incorporating Adaptive Human Behavior into Epidemiological Models using Equation Learning

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Abstract

Mathematical models have proven to be valuable tools for forecasting and evaluating public health interventions during epidemics, such as COVID-19. Covasim is an open-source agent-based model (ABM) recently developed to simulate the transmission of COVID-19. Covasim has been validated with real-world data and utilized for simulating the potential effect of public health interventions. While Covasim’s base model does not implement adaptive behaviors, we can leverage its flexibility to generate data for scenarios where agent behavior can adapt based on the current state of the model, subsequently affecting the epidemic. Human behaviors, such as compliance to masking guidelines, have been shown to depend on the state of the epidemic and can significantly impact disease spread. We extended the Covasim model to incorporate adaptive masking behavior to investigate its effect on the system’s behavior, complexity, and our ability to obtain a mathematical model that accurately captures the dynamics of the extended ABM. Using an existing compartmental model, we processed the data generated from this extended ABM through Biologically-Informed Neural Networks (BINNs) and sparse regression techniques to estimate parameters and obtain an ordinary differential equation (ODE) approximation of this model. The extended ABM and equation learning computational pipeline we developed is open-source to provide a quantitative framework for incorporating adaptive behaviors into forecasting future epidemics and other similar computational models.

1 Introduction

Epidemics present a multi-faceted challenge characterized by highly complicated and intricate interactions between individuals and a disease within a dynamic population. In addition to the system of individuals that a disease spreads throughout being highly complicated, the population that the epidemic affects is comprised of individuals that act adaptively (or maladaptively) to the state of the disease and the epidemic as a whole. This additional aspect significantly increases the difficulty of accurately modelling disease spread and necessitates novel approaches that capture both the individual-level interaction and the emergent dynamics of the population.

Traditional epidemiological models, while providing valuable insights, often struggle to account for individual-level heterogeneity and dynamic adaptation. They typically rely on compartmental models that represent the population in aggregate states, such as susceptible, infected, and recovered (SIR) [1]. While these models offer a simplified view and can be computationally efficient, they often lack the necessary granularity to capture the nuances of individual responses and their impact on the overall epidemic trajectory.

Agent-based models (ABMs) and other computational models offer unique advantages over traditional modelling approaches. ABMs excel at capturing complex system dynamics driven by individual-level interactions, heterogeneity, and emergent behavior, providing valuable insights into real-world phenomena [2]. These benefits extend to various fields, including biology [3], public health [4], and social sciences [5]. However, computational models also face limitations. Despite their ability to represent intricate systems, they can be computationally expensive, particularly with increasing complexity [6, 7]. Additionally, model validation and ensuring biological plausibility can be challenging tasks [8, 3, 6]. Furthermore, analyzing outputs from complex models often requires advanced statistical techniques and careful consideration of variance and sensitivity [7]. Balancing these advantages and disadvantages is crucial when choosing the appropriate computational model for a specific research question.

To address these limitations from both traditional mathematical models and computational models, our research explores the potential of using equation learning as a tool that bridges the insights from each approach under the context of systems with adaptive behaviors. By leveraging ABMs to simulate the complex dynamics of the epidemic and then applying equation learning techniques, it is possible to extract a set of governing equations that capture the essence of the system's behavior [8]. This approach offers several advantages, including:

- Reduced computational complexity: The resulting set of equations can be significantly more efficient to solve than running an ABM, making it possible to perform simulations capable of meaningful extrapolation and analyze scenarios more quickly.
- Increased interpretability: The explicit equations provide a clearer understanding of the relationships between key variables and the underlying mechanisms driving the epidemic's progression and its various defining parameters, such as contact rate.
- Predictive power: The equations can be used to make predictions about the future course of the epidemic and assess the potential impact of different control interventions.

Combining the strengths of agent-based modelling and equation learning holds significant promise for advancing many different fields similar to epidemiology. This approach is particularly powerful when considering the adaptive behaviors of individuals within the population, as it allows data-driven inferencing to obtain a more accurate representation of the complex interactions that shape the course of an epidemic. By offering a more realistic and tractable approach to disease modelling, this framework has the potential to improve our understanding of epidemic dynamics and contribute to the development of more effective control strategies.

2 Related Works

In this section we review approaches towards obtaining an ODE approximation from an ABM using equation learning and parameter estimation.

2.1 Learning Differential Equations from Stochastic ABMs

Nardini et al. [8] propose a novel approach for inferring differential equation (DE) models directly from stochastic agent-based model (ABM) simulations. This method leverages equation learning, overcoming limitations of traditional approaches like Monte Carlo simulations or coarse-grained models. Recognizing the limitations in analyzing complex and stochastic ABM dynamics, the authors utilize equation learning to avoid extensive simulations while still being able to capture the full complexity of ABM dynamics. Their approach successfully infers differential equations from two example ABMs, demonstrating accurate predictions of ABM dynamics and improved computational efficiency compared to classical methods [8].

2.2 BINNs Guide Mechanistic Modelling

The 2020 paper "Biologically-informed neural networks guide mechanistic modelling from sparse experimental data" by Lagergren et al. [9] explores a novel approach to overcoming limitations in traditional methods for learning mechanistic models. These methods often require extensive data and prior knowledge of the underlying mechanisms, which can be limiting in various research fields. They introduce Biologically-Informed Neural Networks (BINNs), which combine parameter approximating neural networks with physics-informed neural networks (PINNs). PINNs are adept at approximating solutions to partial differential equations (PDEs), allowing them to provide good approximate solutions in order to learn the parameters of interest while minimizing *a priori* assumptions (further details in 2.2). We use the framework laid out by Lagergren et al. to infer nonlinear parameters in order to obtain a mathematical model that is capable of simulating a system with adaptive elements. This particular approach of inferring mathematical models from stochastic agent-based models is unique, and although our data is not sparse or experimental, we provide insight into emerging techniques in equation learning while utilizing agent-based models as a tool for simulating a system with adaptive elements.

3 Modelling and Equation Learning

3.1 Our Agent-Based Model: Covasim

Covasim, an agent-based simulator created by the Institute for Disease modelling (IDM), offers a valuable tool for simulating and studying disease dynamics [10]. Covasim's features are easily extended and adapted by users to tailor the simulation to specific diseases and scenarios. However, the existing model lacks a key element: adaptive behavior of agents.

3.2 Incorporating Adaptive Behavior: Masking

We define an adaptive behavior of an agent to be any action that is dependent on the state of the system it resides in. Typically, this behavior will also have an effect on the dynamics of the system, creating a feedback loop between the system and the agents' behaviors. Since adaptive behavior makes actions of agents dependent on the actions of other agents, it directly violates the mean-field assumption making coarse-grained methods far less effective [8].

In real-world disease outbreaks, individual behavior dynamically adapts based on the perceived threat and evolving conditions of the epidemic. This feedback loop between individual actions and the overall system dynamics significantly impacts disease spread and control strategies [11]. We address this by introducing adaptive masking behavior into the Covasim framework. Masking significantly affects disease transmission and is highly dependent on the perceived severity and prevalence of the epidemic [12]. Thus, incorporating this adaptive behavior is essential for achieving a more realistic and accurate model of disease spread.

We introduce a probabilistic masking model based on the diagnosed (D), fatalities (F), and time (t) variables. Intuitively, the probability of masking is expected to be:

- Increasing with D and F : As the number of diagnosed cases and fatalities increase, the perceived threat rises, motivating individuals to adopt masking behavior.
- Decreasing with t : Over time, complacency may set in, leading to a decrease in masking behavior even as the epidemic persists.

We use the logit function with D, F, t as explanatory features to model this adaptive behavior. Our probability of masking for each agent is:

$$p_M = \mathbb{P}(\text{masking}|D, F, t) = \frac{e^{\beta_0 + \beta_1 \frac{D(t) + F(t)}{N} + \beta_2 t}}{1 + e^{\beta_0 + \beta_1 \frac{D(t) + F(t)}{N} + \beta_2 t}} \quad (1)$$

where $\beta_0, \beta_1, \beta_2$ are hyperparameters summarized as follows:

- $\beta_0 \in \mathbb{R}^+ \cup \{0\}$: Represents the initial proportion of the population masking

Compartment	Description	Parameter	Description
S	Susceptible	$\eta(S, A, Y)$	Contact Rate
T	Quarantined and susceptible	$\beta(S + A + Y, \chi)$	Tracing Rate
E	Exposed	$\tau(A, Y)$	Quarantined Diagnosis Rate
A	Asymptomatic and infected	p	Asymptomatic Probability
Y	Symptomatic and infected	γ	Infection Rate
D	Diagnosed and infected	α	Unquarantining Rate
Q	Quarantined and infected	λ	Recovery Rate
R	Recovered	δ	Fatality Rate
F	Fatality	χ	Tracing Interaction (Piecewise)

(a) Compartments of the STEAYDQRF model we use to model Covasim.

(b) Parameters of the baseline ODE system.

- $\beta_1 \in \mathbb{R}^+$: controls the sensitivity of masking behavior to the epidemic's severity.
- $\beta_2 \in \mathbb{R}^-$: dictates the rate of decrease in masking behavior over time.

Each agent then has a corresponding binary random variable $\mathcal{M}(t)$ where

$$\mathcal{M}(t) = \begin{cases} 1 & \text{If masking at time } t. \\ 0 & \text{If not masking at time } t. \end{cases} \quad (2)$$

And has probability mass function

$$f_M(k; p_M) = \begin{cases} p_M & \text{If } k = 1. \\ 1 - p_M & \text{If } k = 0. \end{cases} \quad (3)$$

When $\mathcal{M} = 1$ at time step t within the simulation, for any given agent, we reduce the effective infection rate across each network layer of the corresponding agent within Covasim to model the effect masking has on reducing the spread of disease [12].

3.3 Mathematical Model

We then use an existing compartmental model consisting of 9 different states to mathematically model the spread of disease in the simulation and utilize equation learning methods in order to infer certain parameters of our system of equations. Our base model includes three parameters, contact rate (η), tracing rate (β), and quarantine diagnosis rate (τ), that we suspect to be nonlinear functions which we wish to estimate via neural networks (details in Section 2.2).

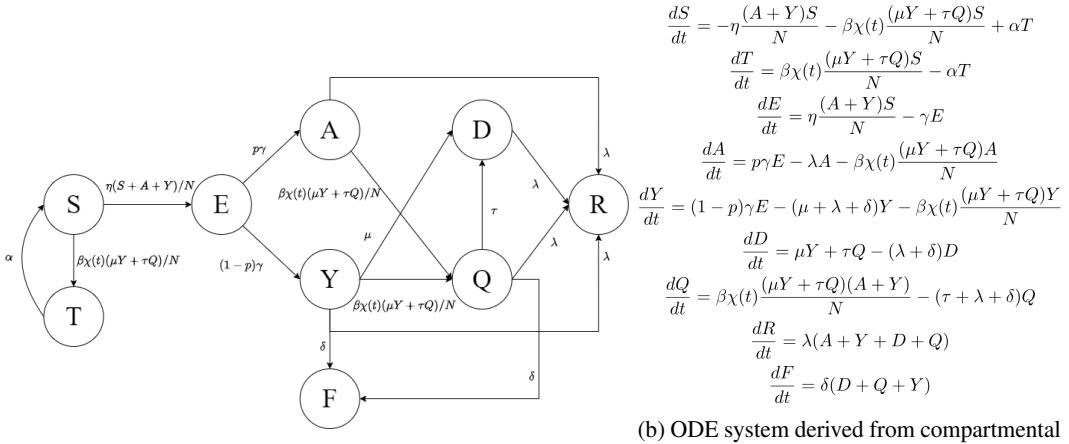


Figure 1: Summary of the base mathematical model we use to model Covasim.

We hypothesized that introducing such adaptive behavior(s) increases the nonlinearity and complexity of the learned equations. In the Results section we demonstrate and confirm this. Additionally, our implementation of masking directly interacts with and decreases transmissibility of the disease. Therefore, it is very likely that in the ABM with adaptive behavior, the dynamics of the contact rate (η) are affected and explained by the proportion of the population masking, M , in addition to S, A, Y as assumed in the original model. Because of this, we augment the existing compartmental model to include a non-mutually exclusive compartment representing the proportion of the population masking, M , as shown in Figure 2. Therefore, using sophisticated techniques in order to accurately learn parameters such as contact rate, tracing rate, and quarantined rate, is vital to the accuracy and interpretability of the learned system of equations. We used Biologically-Informed Neural Networks (BINNs) in order to do this. For data generated with masking as an adaptive behavior, we include the proportion of population masking as an input into the contact rate parameter.

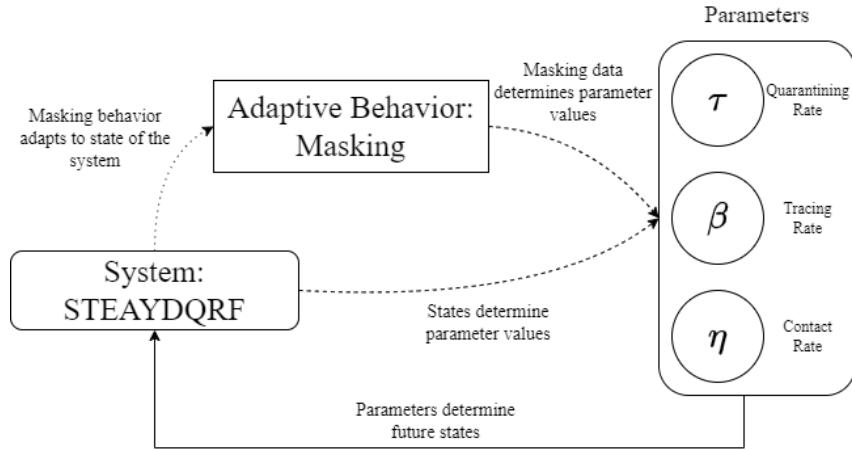


Figure 2: Flowchart diagram illustrating the feedback loop between the states of the system, the adaptive behavior (masking), and the parameters of our model.

3.4 Biologically-Informed Neural Networks for Parameter Estimation

Biologically-Informed Neural Networks (BINNs) attempt to tackle the *model specification problem* by using neural networks as surrogate models to approximate unknown and possibly nonlinear parameters in order to minimize *a priori* assumptions about the form of the differential equation(s) as well as expand the number of possible solutions to such a model [9]. The architecture is split into two key parts. The first is the Biologically-Informed Neural Network that approximates the solutions to the governing dynamical system. The second part consists of the parameter networks that take as inputs the approximated solutions from the biologically-informed part [13]. These parameter networks approximate parameters that provide solutions of our governing dynamical system. Physics-Informed Neural Networks, first introduced in 2018, primarily tackle the issue of inferring a surface of solutions to a system of differential equations. This inherently requires prior knowledge and assumptions of the governing dynamics. One of the most apparent assumptions, which is directly addressed by [9] and mentioned in [14], is the form of each of the parameters in the governing system of equations. Generally, these parameters may be linear, nonlinear, or constant functions. If they are nonlinear, the space of possible functions is too large to accurately solve for without making large assumptions using methods of sparse regression. Hence, using a universal function approximator (such as an MLP [15]) allows us to learn these nonlinear components and then use equation learning with feature selection to infer underlying relationships and functions *a posteriori*.

The architecture of the BINN is primarily dependent on 2 things. 1) What mathematical model we are using. This decides what is inputted into the informed neural network, how the loss function is constructed, and what is outputted (the solutions to the model). 2) The parameters we wish to estimate. Various parameters may or may not need estimation via parameter networks. It is up to the modeller to decide what parameters are worth approximating via parameter networks and which others can be estimated using other methods or are already known. We utilize a BINN that follows

the blueprint discussed and shown in [9]. We approximate η , β , and τ with parameter networks $\hat{\eta}_{NN}$, $\hat{\beta}_{NN}$, and $\hat{\tau}_{NN}$.

Because, as we will later show in Section 4, incorporating certain adaptive behaviors such as masking into our model drastically changes the dynamics, we include observed data of masking into the contact rate parameter in order to obtain more accurate dynamics from our mathematical model.

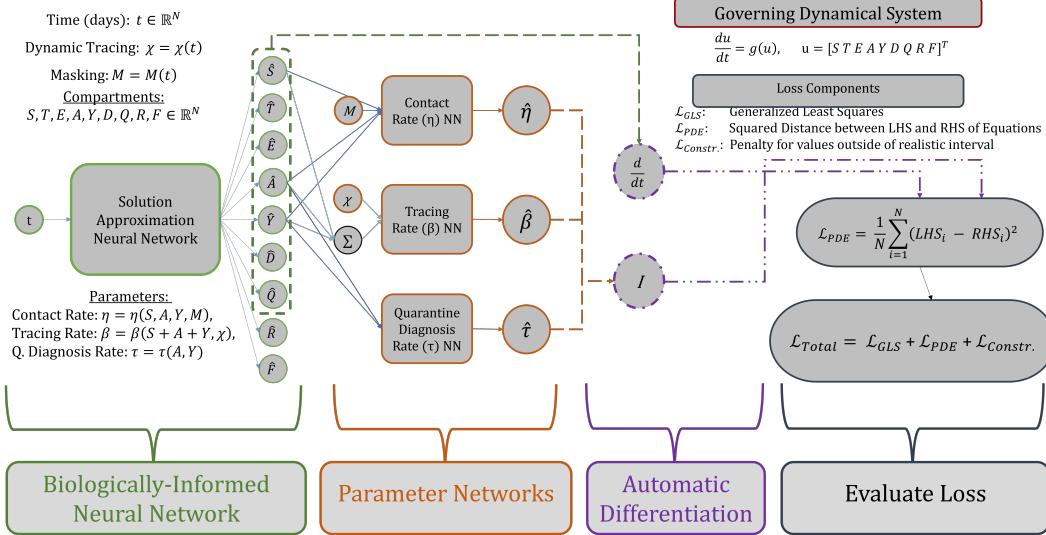


Figure 3: Schematic of our Biologically-Informed Neural Network model for our epidemiological model with masking data as input into the contact rate parameter (η). Note that M corresponds to observed masking data. Σ represents the sum of the inputs ($S + A + Y$). See Lagergren et al.’s 2020 paper for further details on this architecture [9].

3.5 Equation Learning

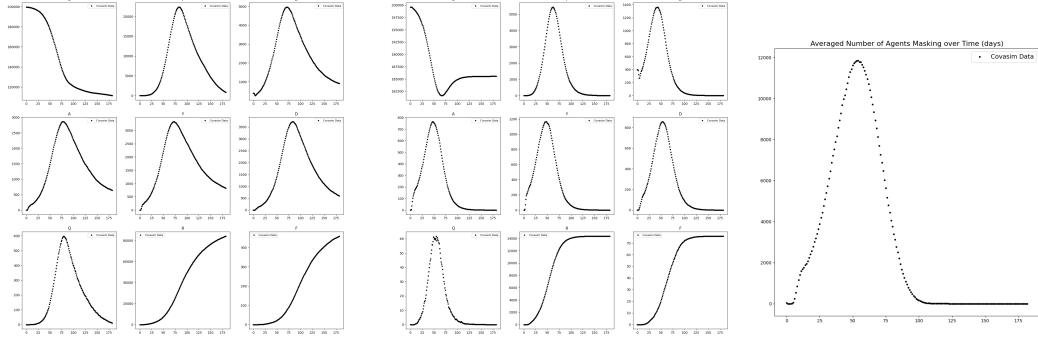
Approximate parameters via BINNs are trained neural networks which we refer to as parameter networks. These parameter networks are non-interpretable function approximations. Although they can provide good approximations of non-linear functions, they do not provide mathematical insight into the dynamics of the parameter it is approximating. That is, they don’t grant insight into the dynamics of the system or our parameter and they cannot provide an approximate closed system of equations for our system in a concise manner (of course, we could express these parameter networks as a composition of functions and affine transformations but they are not very interpretable).

We can use supervised learning techniques to approximate these parameter networks in terms of the space of various interaction terms and functions of its inputs. Specifying this library of terms to act as the basis of this learned equation is done using expert knowledge and intuition of the parameter we wish to estimate. Since the parameter network is a function of specific inputs, we restrict our library to consist of those inputs. In order to ensure a parsimonious learned equation, we use sparse regression methods, specifically LASSO regression due to the sparsifying effect of L^1 regularization and its feature selection capabilities [16].

4 Results

4.1 Effects of Adaptive Behavior on ABM

Adding adaptive behavior into the agent-based model significantly impacted the dynamics of the system. The model exhibited significantly different behavior in each compartment (most notably, the susceptible compartment), as seen in 4b when compared to 4a.

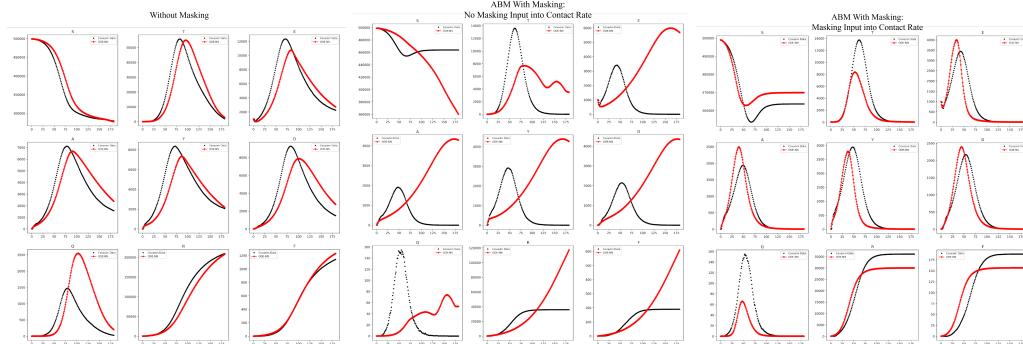


(a) Data generated from Covasim ABM with no masking behavior. (b) Data generated from Covasim ABM with masking behavior. (c) Averaged proportion of population masking over each day.

Figure 4: Comparison between data generated by Covasim without (left) and with (middle) adaptive masking behavior (right).

4.2 Approximate System of ODEs with Neural Networks

We employed BINNs to obtain effective approximations of our parameters of interest via parameter networks. These trained parameter networks effectively capture the dynamic behavior of the parameters and provide solutions that are capable of accurately modelling Covasim with no adaptive behaviors, as seen in Figure 5a. However, after introducing masking into Covasim, our implementation of BINNs was incapable of learning parameter networks that sufficiently model the dynamics of the system, as seen in Figure 5b. To combat this, we then included masking data as a feature of the contact rate parameter network ($\hat{\eta}_{NN}$). This simple modification to our BINNs implementation provided dramatic improvements in the approximate ODE system's ability to model our augmented ABM, as seen in Figure 5c.



(a) Comparison between Covasim data without adaptive masking behavior and Covasim data with adaptive masking behavior. (b) Comparison between Covasim data with adaptive masking behavior and the solutions of an ODE and the solutions of an ODE approximation with parameter networks. (c) Comparison between observed data and the solutions of an ODE approximation with parameter networks without masking data inputted into the contact rate parameter network $\hat{\eta}_{NN}$.

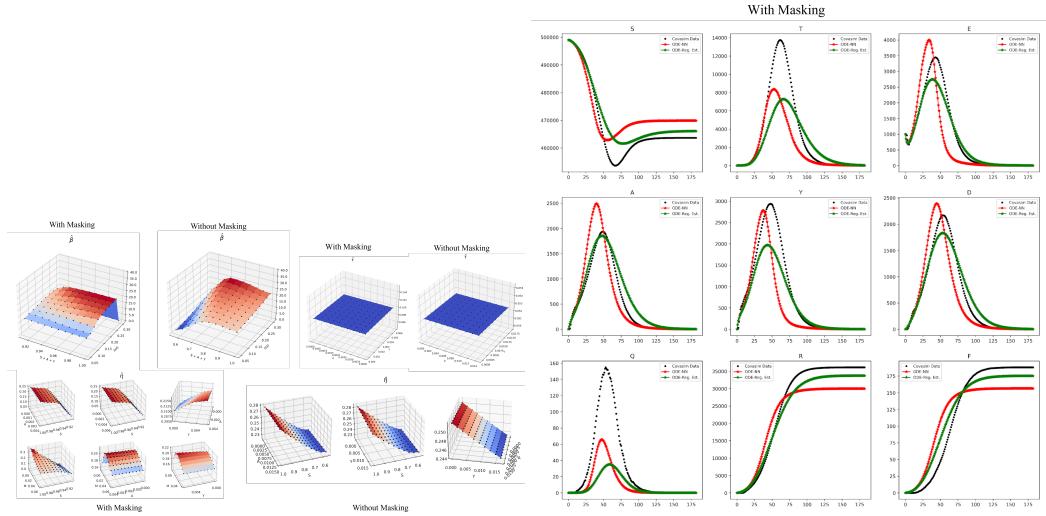
Figure 5: Comparison between observed data (black) and solutions of ODE approximation (red) with parameter networks $\hat{\eta}_{NN}$, $\hat{\beta}_{NN}$, and $\hat{\tau}_{NN}$.

We added masking data as an additional feature to our contact rate parameter because we hypothesized that without any knowledge of masking within the population, the base mathematical model was not able to capture the dynamics of the spread of disease throughout the simulation (as seen in Figure 5). We believed it was likely that certain parameters of the model are directly affected by masking. Specifically, since our implementation of masking affects the effective infection rates for agents across each of their network layers, we believed that masking would affect the contact rate parameter

Parameter	Features with Non-zero Coefficients	MSE
η	$S, A M, S^2, SY, SM, SA, M^2, S^2M$	$9.24536 \cdot 10^{-5}$
β	$S + A + Y, S\chi, (S + A + Y)^2$	$3.921 \cdot 10^{-7}$
τ	None	0

Table 2: Selected features after performing equation learning with LASSO regression on parameter networks. Mean Squared Error (MSE) is measured as the raw MSE between the parameter network and the inference equation.

the most. Therefore, we take observed masking data throughout the simulation at each timestep and feed it as an input into the contact rate parameter network, now making our contact rate a function of S, A, Y and M . This incorporation of adaptive behavior led to a drastic increase in the complexity and nonlinearity of the model’s parameters, as demonstrated by Figure 6a.



(a) Comparison of surfaces of our parameter networks when trained on Covasim without masking (and no masking behavior, solutions to ODE system with parameter input into contact rate) and Covasim with parameter networks, and solutions to ODE system with masking (with masking input into contact rate). (b) Comparison between observed Covasim data with inferred equations approximating parameters.

Figure 6: Obtained parameter networks with masking adaptive behavior and their corresponding solutions to our ODE system.

4.3 Closed System of ODEs Through Equation Learning

By performing equation learning on the neural network, we obtained a closed approximate system of ODEs that modeled the entire agent-based model, including the adaptive behavior. This system offers several advantages: analytical tractability, allowing us to perform analytical calculations and utilize established mathematical tools to further investigate the system’s dynamics; computational efficiency, requiring significantly less computational resources than running the full agent-based model, enabling faster simulations and parameter optimization; and increased interpretability, providing a clearer understanding of the relationships between key variables and the underlying mechanisms driving the system’s behavior.

5 Discussion

This study explored the potential of merging agent-based modelling (ABM) and equation learning to study complex systems with adaptive behavior. Utilizing Covasim, we simulated an epidemic with adaptive masking behavior, demonstrating the significant impact of individual-level behavior on disease dynamics [2]. Biologically-Informed Neural Networks (BINNs) proved effective for param-

eter estimation, guiding equation learning to infer an effective approximate system of differential equations [9].

Through equation learning, we successfully extracted a closed system of ordinary differential equations (ODEs) from the trained neural network, offering a simplified and interpretable representation of the ABM's essential behavior [8]. Notably, the original ODE system without masking became insufficient to capture the dynamics when adaptive behavior was introduced. However, augmenting the model with masking data as a feature of the contact rate parameter resolved this issue.

The increased complexity and nonlinearity introduced by the adaptive behavior were evident in the compartment plots seen in Figure 6b and the surfaces of the parameter networks in Figure 6a. This highlights the challenges associated with modelling such systems. Nevertheless, applying equation learning techniques yielded a parsimonious closed-form system of ODEs that approximated the complex parameter networks. This system provides an interpretable and computationally efficient representation of the ABM, capturing the essential dynamics with a reduced number of terms.

This research contributes to the growing field of equation learning and its application to complex adaptive systems. It demonstrates that combining ABMs and equation learning can be a valuable approach to understand the dynamics of such systems and develop accurate and interpretable models.

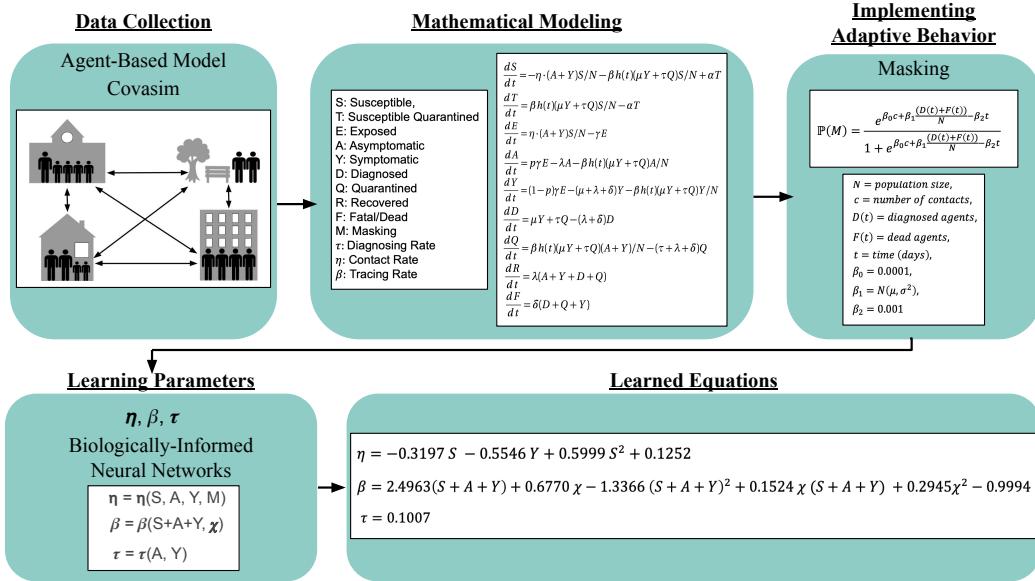


Figure 7: Schematic of the computational pipeline. We start with a base computational model and mathematical model, augment each of them by including adaptive behavior, then perform parameter estimation and equation learning to obtain a closed approximate system of differential equations.

5.1 Limitations

While this study offers promising results, some limitations require consideration. Firstly, the research focused on a single case study involving adaptive masking behavior. Additionally, our method of modelling masking behavior focused on providing a simple but effective modification to our ABM that results in complicated dynamics. Our work does not delve into accurately modelling adaptive behaviors. Further, the accuracy of the inferred ODE system depends on the availability and quality of training data. Larger and more diverse datasets are necessary to improve the generalizability of the learned equations. Finally, the inferred ODE system might still be too complex for certain applications. Future work should focus on developing methods for reducing model complexity while maintaining accuracy.

5.2 Future Work

Despite these limitations, several promising avenues for future investigation exist. One promising direction involves extending the framework to different adaptive behaviors relevant to disease spread, such as social distancing or vaccination uptake. Additionally, integrating domain knowledge into the equation learning process could guide the discovery of parsimonious and biologically plausible models. Analyzing the learned equations to gain insights into the underlying mechanisms driving the system’s behavior and identify potential interventions presents another exciting research opportunity. Finally, creating automated pipelines for generating ABM data, training BINNs, and performing equation learning would make the approach more accessible to a wider range of users.

By addressing the identified limitations and pursuing these promising future directions, we can further enhance the capabilities of equation learning and its application to complex adaptive systems. This will ultimately contribute to the development of improved models for disease prediction and control.

5.3 Conclusions

In conclusion, we successfully obtained an approximate system of ordinary differential equations for an Agent-Based Model with adaptive behaviors. This achievement was made possible by combining neural network approximation with equation learning techniques. The resulting system offers a powerful tool for analyzing and understanding complex adaptive systems, paving the way for further research and applications in various fields.

6 Methods

All methods herein were implemented in Python 3.10.11. We used Covasim 3.1.3 for our agent-based model and all examples of generated data. Deep learning methods used the PyTorch 1.12.1 deep learning platform. Linear regression methods utilized the sci-kit learn machine learning library. Numerical methods were done using SciPy 1.11.1. All data and code are made publicly available at github.com/abarton51/BINNs_EQL_Covasim. The following section is intended to provide an outline for the computational pipeline we developed and how to adapt it to a wide range of agent-based models. Specifically, this section covers (i) how to model an adaptive behavior and add it into an agent-based model, (ii) choosing a mathematical model and the importance of making necessary changes to it for the adaptive behavior, (iv) the basic architecture of the corresponding BINN, (v) evaluating trained parameter networks, and (vi) inferring equations using sparse regression.

6.1 Adaptive Behavior

We chose masking as our adaptive behavior because of its proven effects of reducing disease spread [17, 12]. We chose the logit function because of its simplicity and interpretability. Further improvements on modelling the adaptive behavior itself can be made, but our work focused on demonstrating drastic effects on an ABM when introducing adaptive behavior to more accurately model disease spread, and then utilize a data-driven approach to obtaining an ODE approximation.

6.2 The Mathematical Model

The mathematical model selected should be sufficiently accurate enough to model the complex system so long as the parameters are approximated well enough. Each mathematical model has a limit to how accurate it can model certain complex systems. Using simple mathematical models to model highly complex systems will often result in poor results even with the most optimal parameters in the system. Deriving more sophisticated models is a daunting and challenging process which heavily depends on accurately portraying dynamics of certain parameters, such as contact rate in disease spread. If the model is not interpretable, then the likelihood of human error in creating the BINN model, evaluating, and/or performing equation learning is much higher.

6.3 Evaluation Procedure

Parameter networks are trained in the BINN to provide solutions that are close to the approximated solutions. Additionally, the loss between the left and right hand sides of the equations is almost never

0. Therefore, the solutions of the system with the trained parameter networks as surrogate models may be vastly different from the observed data. In order to evaluate the trained parameter networks and see if they provide solutions to our system of differential equations that accurately model our system, we plug them into the RHS of the system of equations and numerically solve. We utilize the Runge-Kutta-Fehlberg method (RK45). Once approximated solutions are obtained, we visually compare them to the observed data. Further analysis on the accuracy of this model can be done but for our intents and purposes, a visual inspection is sufficient.

6.4 Equation Inferencing

Parameter networks may provide an accurate mathematical model, but they lack interpretability and do not provide a closed system of equations that models the system. We utilize sparse regression on a feature space of interaction terms of inputs of the parameters up to a certain degree to obtain an equation that estimates these surrogate parameter functions. Since this process almost guarantees some error, re-evaluation on these inferred equations must be done in order to verify the validity of the learned system of equations.

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A Supplementary Material

A.1 Code Repository

All code for this project was implemented in Python and is open-source. Code repository can be accessed through this link: https://github.com/abarton51/BINNs_EQL_Covasim.