Deep Learning-based Spatially Explicit Emulation of an Agent-Based Simulator for Pandemic in a City

Extended Abstract

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ABSTRACT

Agent-Based Models are very useful for simulation of physical or social processes, such as the spreading of a pandemic in a city. Such models represent the behavior of individuals (agents) and their interactions, based on the geography and demography of the city, and the resulting spread of infections. However, they are computationally very expensive. This seriously limits the usage of such models for simulations, which often have to be run hundreds of times for policy planning and even model parameter estimation. An alternative is to develop an emulator, a surrogate model that can predict the Agent-Based Simulator's output based on its initial conditions and parameters. In this work, we propose a Deep Learning model, based on the Dilated Convolutional Neural Network, that can emulate such an Agent-Based Model with high accuracy. We show that use of this model instead of the original Agent-Based Model provides us major gains in the speed of simulations, allowing much quicker calibration to observations, and more extensive scenario analysis. The models we consider are spatially explicit, as the locations of the infected individuals are simulated instead of the gross counts. Our framework uses a divide-and-conquer approach that divides the city into several small overlapping blocks and carries out the emulation in them parallelly, after which these results are merged together. This ensures that the same emulator can work for a city of any size, and also provides significant improvement of time complexity of the emulator, compared to the original simulator.

KEYWORDS

Agent-based models; Epidemiology; Convolutional Neural Network

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1 MOTIVATION

During the Covid-19 pandemic throughout 2020-2021, it was necessary to make a delicate trade-off between curbing disease spread and socio-economic disruption due to Non-Pharmaceutical Interventions (NPIs) like lockdown orders. This needed an estimate of the possible consequences of different policies, or a *what-if* analysis. Epidemiological Models gained considerable attention for this purpose. While *differential equation-based compartmental models* like SEIR [1] are fast and simple, they do not specifically represent how people interact, based on the geographic and demographic factors of a city. An alternative approach is that of *stochastic agent-based models*, which represent the attributes, activities and interactions of individuals (considered as agents). This type of models have earlier been used in the domains of computational social science [5, 8], urban systems [18], economics [23], ecology [10] and population biology [7]. Works such as Fosset et al. [9], Hager et al. [11], Huynh et al. [14], Kagho et al. [15], Patel et al. [19], Waddell et al. [25] have focused on simulation of different aspects of urban life. In the context of the Covid-19 pandemic, a number of agent-based models were developed for specific regions [12, 13, 16, 21, 24]. These models use varying levels of details in the representation of geographical and social aspects of their regions of focus. In general, a more detailed model requires more data and computations, but should produce more realistic simulations. As these simulations become more expensive with more details, it is important to develop surrogate models or emulators [2–4, 26] that can predict simulation outputs from initial conditions, without running the simulation.

2 AGENT-BASED PANDEMIC SIMULATION

We consider a city divided into K blocks. The blocks have populations $N_1, N_2, \ldots, N_K$ such that $\sum_{k=1}^{K} N_k = N$. Each resident i has attributes like age, family connections, health status and workplace, and mapped to a residence block S_i. A pandemic strikes the city with basic reproductive number $R_0(t)$ on day t (this index varies over time as the virus mutates and NPIs are put in place). At t=0, I_0 people are infected, who may belong to any block uniformly at random. Over the days, the infections spread, and on day t, X_{kt1} people in block k are infected, X_{kt2} persons recover there, X_{kt3} persons are hospitalized etc. This number depends on the social interactions among the people and the NPIs imposed, like total or partial lockdown orders. However, an individual may follow orders with compliance rate γ.

We use the agent-based model described in [22], which has a city component including the geographical locations of buildings, educational institutes, workplaces and community spaces. The daily movement of people to these places is simulated. There is also a module to track the infection status of the people (susceptible, asymptomatic, symptomatic etc), and update them stochastically as people interact, using the basic reproductive index R_0. A health module keeps track of the health conditions of the infected people, including detection, quarantining, hospitalization, recovery

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or death, based on pre-specified parameters. The simulation proceeds by stochastic sampling of the variables sequentially. The ABM scales linearly with population and the number of city blocks.

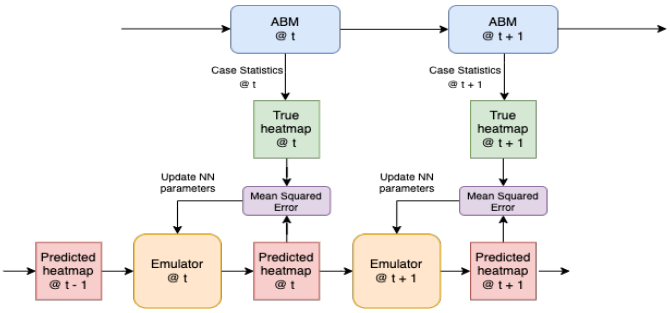

Figure 1: The training procedure of the emulator

3 DEEP LEARNING FOR EMULATION

The simulation by the agent-based model is a multi-channel spatio-temporal sequence $X = \{X_{kti}\}_{k=1,t=1,i=1}^{K,T,L}$ as $X = f(N_0, R_0, \gamma)$. Our aim is to develop a neural network g, which can predict X_{kti} as $\hat{X}_{kti} = g(\{\hat{X}_{jt'l}\}_{j=1,t'=t-H,l=1}^{K,t-1,L}, \{R_0(t')\}_{t'=1}^{t-1}, \gamma)$. Here, H is a time horizon or look-back window. Using this neural network, we aim to predict the full sequence X of daily infections. Clearly, this is a spatio-temporal prediction problem.

The surrogate model takes as input at each time step 1) the simulation parameters (initial number of infections (at $t = 0$), compliance rate γ, and Basic Reproductive Number $R_0(t)$), and 2) the past spatio-temporal heatmap sequence. Using this input, the model predicts the subsequent heatmap sequence over the next time steps. After each time step the model is fed its own predictions back as inputs at the next time step. The model is trained to minimize the Mean Squared Error (MSE) between the predicted heatmaps (i.e. model output) and the actual heatmaps (i.e. ABM predictions). This way a complete prediction of the heatmap sequence is generated by the emulator, as illustrated in Figure 1.

We experimented with several network architectures for the emulator, such as ConvLSTM [20]. The best results were obtained from a 2D version of the Dilated CNN [6], that uses stacks of convolutional layers with increasing dilations, allowing it to access data from past time steps.

4 ACCURACY AND EFFICIENCY

The training data for emulator is generated by running the ABM with different values of parameters like *Reproduction Number* (R_0), initial infected population N_0, lockdown duration and compliance ration γ are varied to generate distinct series. We consider a city with a population of $N = 100000$ residents, distributed over a 20x20 gridded block structure, and run simulation for $T = 100$ days. R_0 is varied between 1 and 4 in steps of 0.1. 3 case-statistics are tracked each day at each block: - *Cumulative Positive Tested*, *Current Hospitalizations* and *Current Asymptomatic Free*. We split these sequences into training, validation and testing sets in the ratio 80:10:10 (410 + 51 + 51), uniformly across all parameter values. The lookback window size for the emulator is $H = 5$. To evaluate the emulator, we compare the time-series of the 3 aforementioned statistics as generated by the Agent-Based Model against those predicted by the emulator. The plots from our emulator are much closer to the ABM's plots compared to another recent neural network based emulator [3]. We also examine the spatio-temporal heatmap sequences generated by the ABM and compare them against the predictions by the emulator.These heatmaps closely match the heatmaps obtained from the simulator. The emulator can also reproduce simulation results with unseen values of R_0. But it struggles if R_0 is close to 1.

Task	Simulator	emulator
20x20 city-grid simulation time	38.0626 sec	
emulator training		503.93 sec
inference (10x10)		0.75 sec
scaled inference (20x20)		0.76 sec

Table 1: Times required (in seconds) to generate complete trajectories by simulator and emulator

The aim of the surrogate model is to reproduce the Agent-based Model's simulation with high accuracy in significantly less time. We use the parallel computing ability of modern GPUs to produce spatio-temporal predictions for large cities using small amounts of training data. Instead of training separate emulators for different block sizes, we can use the same emulator by dividing the city into smaller overlapping regions, carrying out the emulation parallelly in each of them, and combining them by averaging over the overlapping regions. We call this as the *Divide-and-Conquer* framework for emulation. An emulator trained at a particular resolution (e.g. 10x10) can be used to emulate any larger city e.g. 20x20, 30x30, 40x40, etc by this approach. This parallel approach give us significant time-gain, which we show in Table 1. Note that for n simulation runs on a 20×20 city, the Agent-Based Model will require $38n$ seconds, while the emulation will require $504 + 0.76n$ seconds, which gives a major gain especially for high values of n.

In practical applications of epidemic ABMs, we often have historical observations of daily new cases, hospitalizations, recoveries, deaths, etc., but we do not know R_0 or γ. Suitable values of these statistics are usually chosen by calibration, using grid search, Bayesian Optimization, rejection sampling, etc. We experimentally show that Bayesian Optimization can be used to estimate the value of the virus R_0 from data simulated by the ABM, using a randomly sampled value of R_0. The Mean Squared Error (MSE) of this predicted heatmap sequence vs. the ABM's heatmap sequence is used as the objective function. We can also use this approach to simulate possible outcomes in counterfactual scenarios of intervention, such as weekend-only lockdown or ward-wise lockdown. For detailed results, see the full version of our paper [17].

5 CONCLUSIONS

The main drawbacks of the current model is that, the predictions of new cases start failing beyond a time-point, and the accuracy varies with the R_0 value. Further, the emulator is currently able to provide only point estimates, though the agent-based simulations are stochastic. We hope to address these issues in near future.

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