Delft University of Technology
German Aerospace Center & University of Bonn

Project: Graph Neural Network Surrogates to Replace Agent-Based Models for Pandemic Response

Supervisor(s):
Alexander Heinlein (Numerical Analysis, EEMCS)
Martin Kühn (German Aerospace Center & University of Bonn)

March 23, 2025

Topic

During the recent COVID-19 crisis, mathematical modeling has been one of the principal forms to provide evidence on the effectiveness of public health and social interventions [1]. Due to local outbreaks and human contact patterns, infectious disease dynamics are often heterogeneous on a spatial or demographic scale and for efficient mitigation, local transmission dynamics should be integrated in a mathematical model.

Over the last years, a large number of authors has made contributions to predict the development of SARS-CoV-2. Simple ordinary differential equation based models have been used for their efficiency in time-critical moments and through metapopulation modeling, various authors addressed the spatially heterogeneous spread of SARS-CoV-2 very efficiently; see, e.g., [2]. On one hand, these models are very efficient and integrate a meaningful level of complexity, on the other hand, they can not be executed on-the-fly. While a HPC infrastructure can be used to run a parallelized version or to simulate thousands to millions of runs for parameter estimation or scenario considerations in short time, we need to ensure low-barrier access to reliable and up-to-date results for public health experts and decision makers. This is even more important as time is a critical factor in pandemics and evaluations of mitigation and reaction strategies have to be conducted in narrow time windows, with constantly changing initial conditions.

Recently, expert mechanistic modeling were suggested to be combined with AI-based approaches to allow for an on-the-fly execution of reliable and accurate infectious disease models [3]. While the authors' results already provided substantially accelerated surrogate model that performed well on a broad range of tested trajectories, surrogate models for agent-based models (ABMs) need to be studied more in detail. For ABMs, individuals are modeled with a natural and explicit form of human contact behavior. However, switching the original model from a metapopulation approach to an ABM needs an in-depth study of many items. While, first, stochasticity in ABMs adds an additional complexity layer, second, the nature of ABMs means a drastic increase underlying data for the surrogate models to be trained on.

Contact

Are you interested or do you have any questions? Send an email to Alexander Heinlein (a.heinlein@tudelft.nl) and/or Martin Kühn (martin.kuehn@dlr.de).

References

[1] European Centre for Disease Prevention and Control. Public health and social measures for health emergencies and pandemics in the EU/EEA: recommendations for strengthening preparedness planning. Technical report, 2024.

[2] M. J. Kühn and et al. Assessment of effective mitigation and prediction of the spread of SARS-CoV-2 in Germany using demographic information and spatial resolution. *Mathematical Biosciences*, page 108648, 2021. ISSN 0025-5564. doi: https://doi.org/10.1016/j.mbs.2021.108648.

[3] A. Schmidt, H. Zunker, A. Heinlein, and M. J. Kühn. Towards graph neural network surrogates leveraging mechanistic expert knowledge for pandemic response, 2024. URL https://arxiv.org/abs/2411.06500.