# Deep learning of stochastic contagion dynamics on complex networks

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Models of dynamics on networks provide invaluable insights into the underlying mechanics of complex systems. However, as effective as they are to convey understanding of these phenomena, they suffer from two limitations. The first one is the limited quantitative accuracy of their predictions, which is to be expected given that most models are based on a handful of mechanisms that can hardly reproduce the intricacies of real complex systems. One possible solution is then to complexify these models by including more detailed and refined mechanisms. This leads to the second limitation: As further mechanisms are added, models get less mathematically tractable or the estimation of their numerous parameters becomes difficult from limited data. With this in mind, it becomes relevant to explore new tools for complex network modeling.

In this work, we demonstrate the great potential of deep learning to model stochastic dynamics on complex networks. We consider learning effective mechanisms automatically from time series data with a learnable model parametrized by a graph neural network (GNN) [1]. Our contribution is fourfold. First, we design a GNN model which computes the transition probabilities of the system, conditioned on a *known* network structure. Second, we propose a reliable procedure to train the GNN model on finite time series. Third, this allows us to expose a proof of concept of our data-driven approach on synthetic data. We illustrate the performance of our GNN using three stochastic dynamics: A *simple contagion* process (the susceptible-infected-susceptible or SIS model, Fig. A), a *complex contagion* process with a nonmonotonic activation function (Fig. B), and an *interacting contagion* model consisting of two interacting SIS-like diseases. Our results suggest that the accuracy of our GNN predictions is influenced by the topology of the network used to generate the training data—scale-free networks tend to yield more accurate models. Finally, we show that our GNN model, trained on a given network, can be used to project the same dynamics on other networks of arbitrary size and topology. To substantiate this, we use our GNNs to compute the bifurcation diagrams of these spreading models on networks different than the one used for training (Figs. C-D-E). We find that our data-driven approach recovers accurately first and second order phase transitions while requiring minimal fine tuning during training, thus demonstrating the flexibility and the strong potential of this new technique.

[1] Z. Zhang, P. Cui, and W. Zhu, "Deep Learning on Graphs: A Survey", arXiv:1812.04202 (2018).
[2] P. G. Fennell and J. P. Gleeson, "Multistate Dynamical Processes on Networks: Analysis through Degree-Based Approximation Frameworks", SIAM Rev. **61**, 92-118 (2019).

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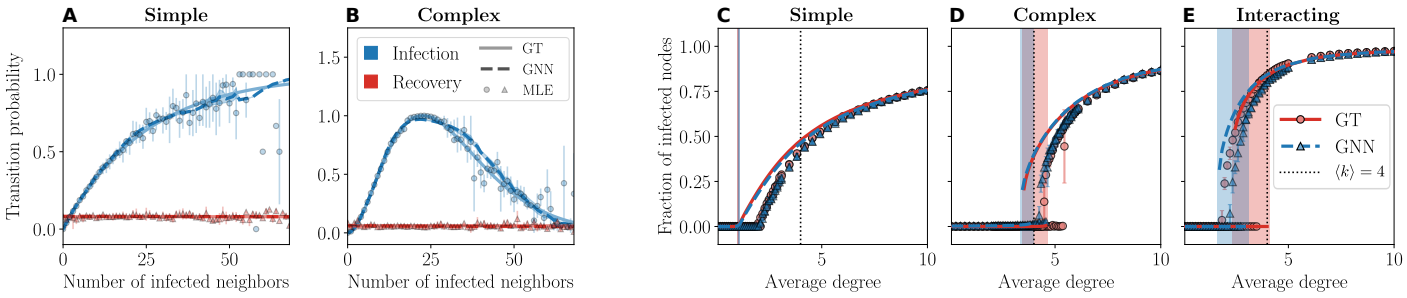


(**A–B**) Local transition probabilities of (**A**) the simple contagion model and (**B**) the complex contagion model as a function of the number of infected neighbors. The known transition probabilities ("ground truth", GT) of the dynamics used to generate the training datasets are shown using solid lines, and the transition probabilities predicted by the GNN are shown with dashed lines. For comparison, we also show the maximum likelihood estimators (MLE) of these probabilities evaluated from the training dataset (symbols). In all cases, the probabilities of infection and of recovery are shown in blue and in red, respectively.
(**C–E**) Bifurcation diagrams for (**C**) the simple, (**D**) the complex and (**E**) the interacting contagion processes. We show the stationary fraction of infected nodes for different random networks of varying average degree and of size $N = 2000$. The symbols correspond to Monte Carlo simulations (50 per symbol) and the lines are predicted with a degree-based meanfield framework [2] which used the "ground truth" transition probabilities (in red) or the ones inferred by the GNN (in blue). Note that the results from the meanfield equations and from the Monte Carlo simulations are not expected to coincide. The accuracy of the trained GNNs can instead be appreciated by comparing the overlap between its predictions and that obtained by using the "ground truth". The thresholds, shown by the vertical colored bands, are numerically computed from this meanfield description. As a reference, we indicate the average degree of the training network with a dotted line to emphasize the versatility of the trained GNN.
(**Training details**) In each experiment, the time series used for training were generated with a Barabási-Albert network of size $N = 1000$ and average degree $\langle k \rangle = 4$. The size of the training dataset was fixed to $10^4$ time steps.