Deep learning of contagion dynamics on complex networks

Murphy, Laurence and Allard

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Key Contributions

- A training procedure and appropriate GNN architecture.
- Assessing validity of the approach.
- Providing predictions for unseen network structures.

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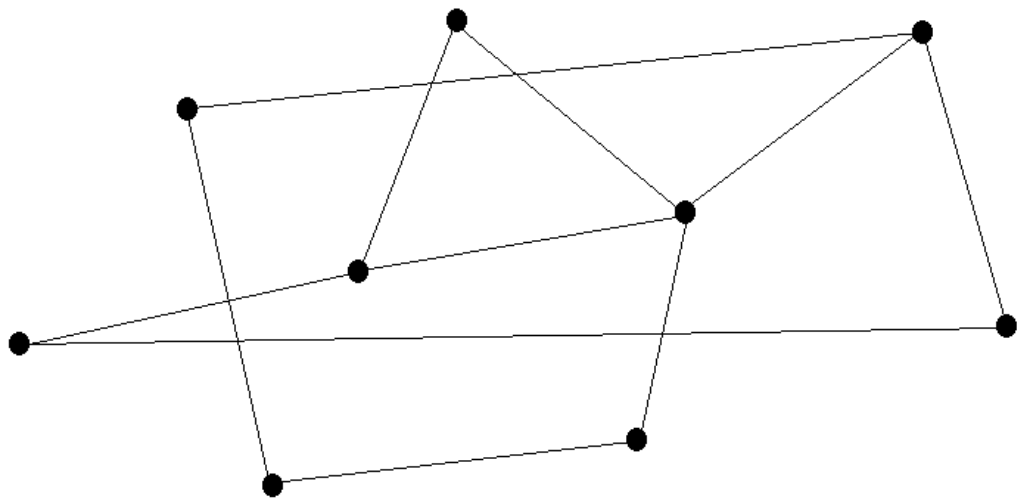

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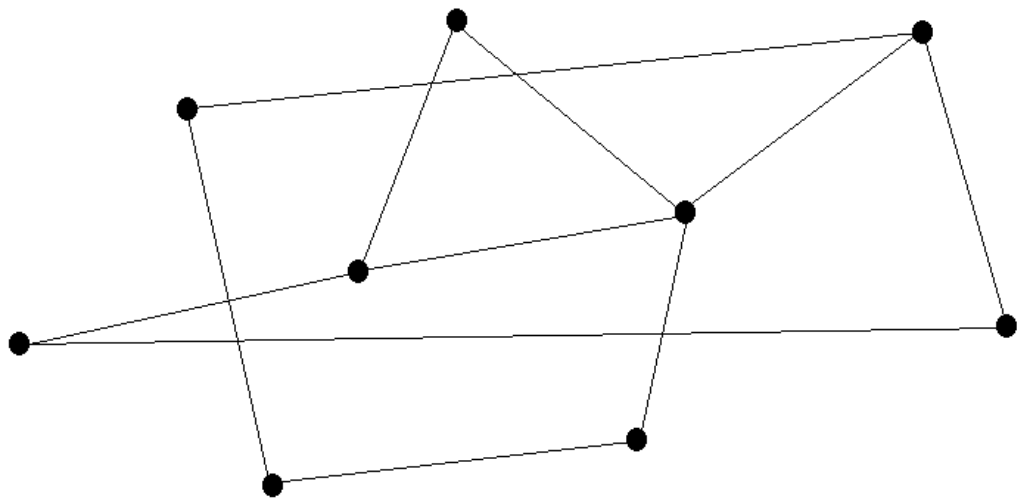

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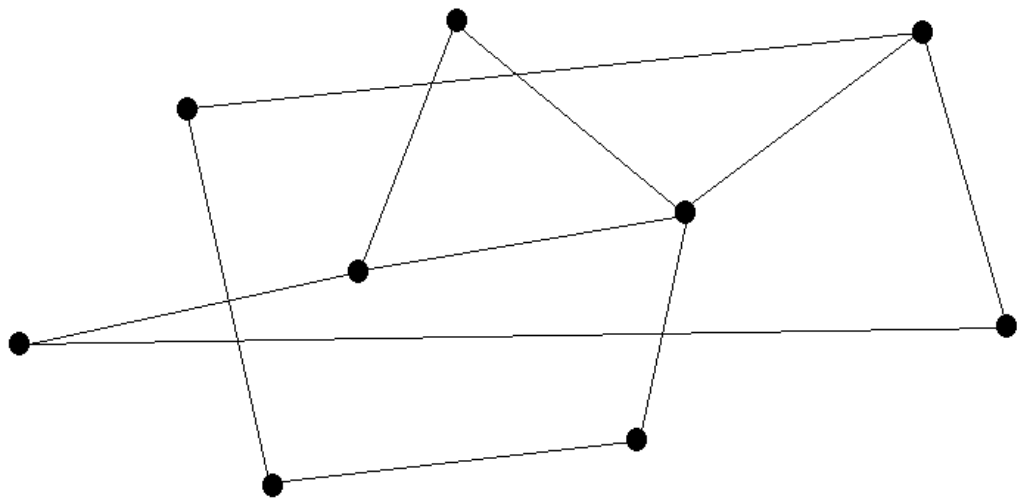

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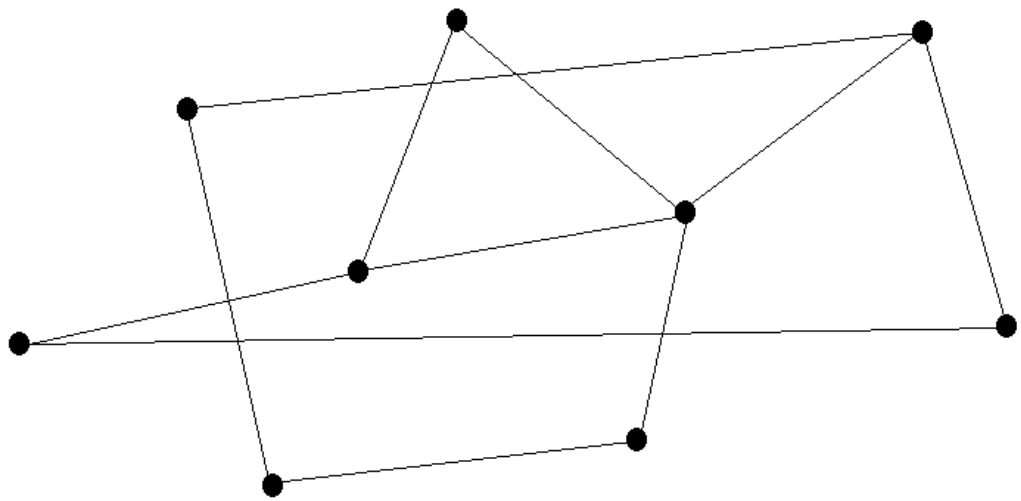

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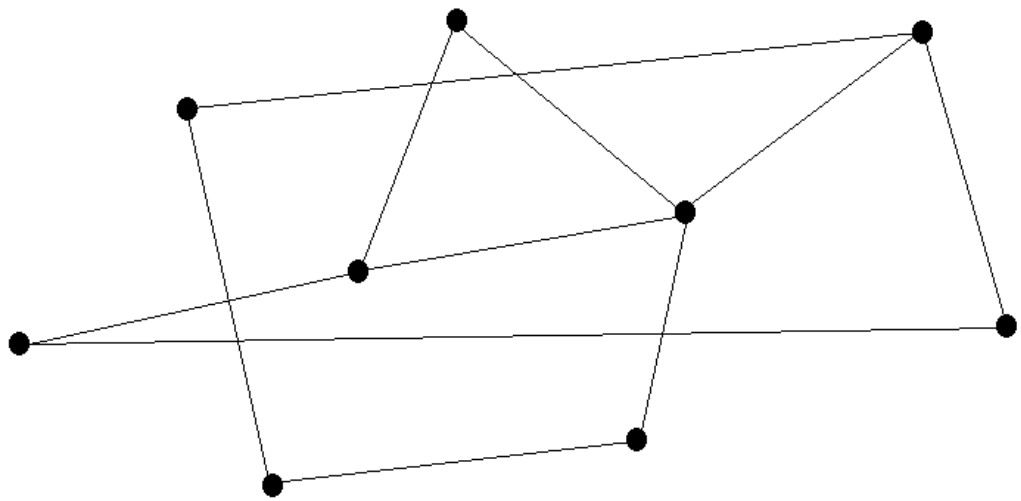

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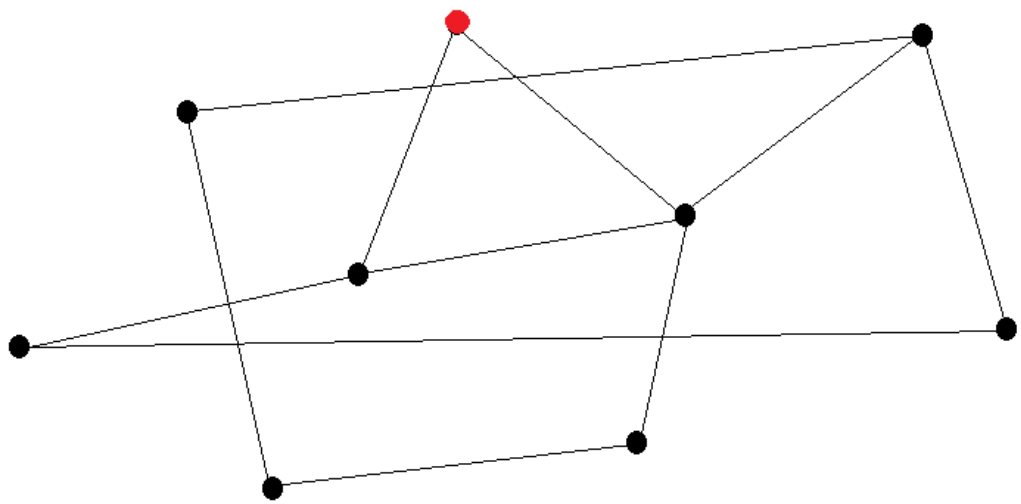

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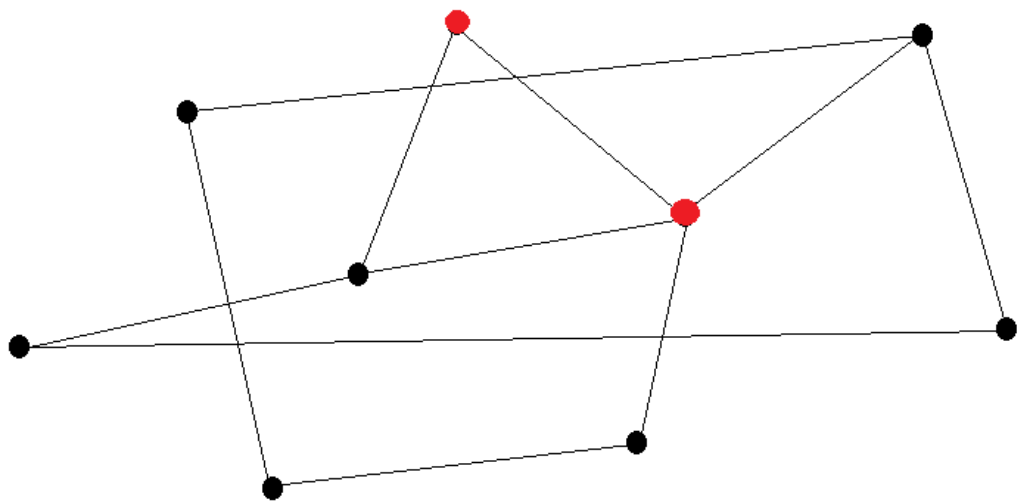

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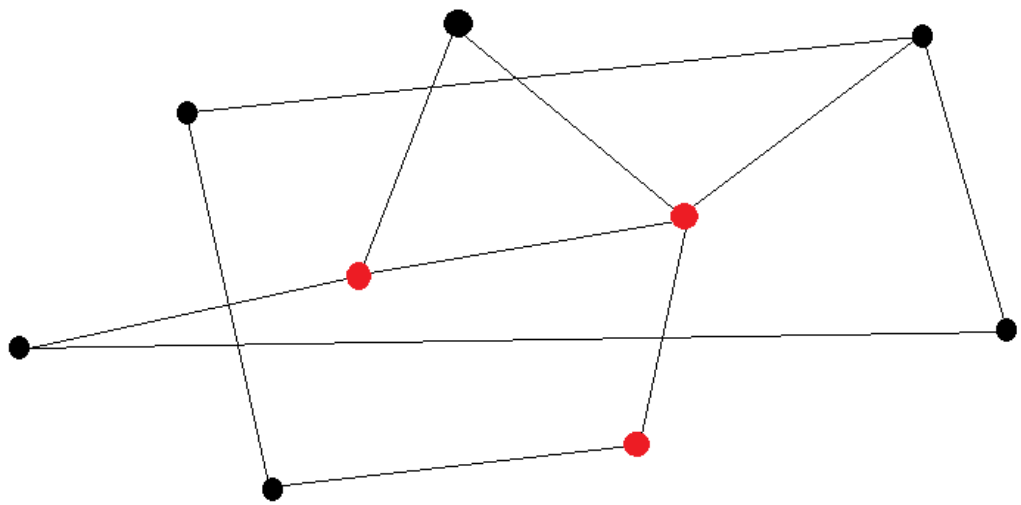

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Therefore, the outcomes from the GNN will be

$$\hat{y}_i = \hat{f}\left(x_i, \Phi_i, x_{\mathcal{N}_i}, \Phi_{\mathcal{N}_i}, \Omega_{i\mathcal{N}_i}; \Theta\right)..$$

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$$w_i(t) \propto \rho\left(k_i, x_i, \Phi_i, x_{\mathcal{N}_i}, \Phi_{\mathcal{N}_i}, \Omega_{i\mathcal{N}_i}\right)^{-\lambda},$$

where k_i is the degree of node v_i in G.

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IV *Metapopulation* dynamics: status of individuals are gathered by geographical regions. E.g. Deterministic metapopulation dynamics with constant population size, and have S, I or R for each individual.

Performance

- We compare GNN predictions $\hat{y}_i(t)$ with corresponding target $y_i(t)$.
- Use Pearson correlation coefficient r between predictions and targets. Compute error as $1 - r$ for each degree class k.
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A **Barabasi-Albert** network is one in which we begin with m_0 nodes fully connected to each other. Nodes are then added one at a time, and are each connected to $m \leq m_0$ existing nodes. A connection with an existing node i is made with probability

$$p_i = \frac{k_i}{\sum_j k_j}.$$

So we tend to see certain nodes become "hubs" and others become relatively isolated.

Performance

A Graphical Interlude

Graph Neural Network Architecture

First transform state of every node, x_i, with shared multilayer perceptron using

$$\hat{f}_{in} : \mathcal{S} \to \mathbb{R}^d$$
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$$\nu_i = \hat{f}_{att}(\xi_i, \xi_{\mathcal{N}_i}) = \xi_i + \sum_{v_j \in \mathcal{N}_i} a_{ij}\xi_j.$$

Other important details

- The rectified Adam algorithm was used to optimise the hyperparameters.
- When $\mathcal{S}$ is discrete and countable, can simplify inputs to $\rho(.)$, which we estimate as

$$\rho(k, x, l) = \frac{1}{|\mathcal{V}|\, T} \sum_{i=1}^{|\mathcal{V}|} \mathbb{1}\left(k_i = k\right) \times \sum_{t=1}^{T} \mathbb{1}\left(x_t(t) = x\right) \mathbb{1}\left(l_i(t) = l\right).$$

- When we have continuous states, we cannot estimate ρ directly, and so we instead use

$$w_i(t) = \left[P(k_i)\Sigma\left(\Phi_i, \Omega_i | k_i\right) \Pi\left(\bar{x}(t)\right)\right]^{-\lambda}.$$