Investigating dynamics of Neural Cellular Automata in complex systems

Vaibhav Mahajan and Soumya Banerjee

University of Cambridge, UK

{vm439,sb2333}@cam.ac.uk

Abstract

Neural cellular automata (NCA) provide a powerful yet still interpretable computational paradigm for modelling morphogenetic processes through local interactions and self-organisation. We apply NCAs to several prototypical complex systems, exploring the capacity of NCA to learn the underlying update rules of dynamic systems solely from spatiotemporal snapshots. We find that NCAs cannot be applied "out of the box" to these diverse problems but must be adapted. We introduce a stratified multi-step training process that can be used to train NCAs to replicate diverse complex systems. Lastly, we find that NCAs use the hidden channels to generalise to novel behaviour. We further analyse the role of hidden channels in encoding spatial memory and guiding complex pattern formation.

Our experiments provide new insights into how neural CA can be adapted as general-purpose models for learning, replicating, and possibly innovating system dynamics. Our findings illustrate the versatility of NCA as a self-organising and rule-learning system (albeit with complex training regimes) and suggest broader applications in modelling natural and artificial systems.

Introduction

The original NCA model demonstrated an impressive capability to self-organise and regenerate patterns. However, it remains an open question whether such models can generalise and be used to infer rules underlying arbitrary spatiotemporal phenomena given only snapshots of the behaviour.

We explore the potential of NCA to learn the dynamics of a system from observation alone. We focus on the morphogenesis system of Mordvintsev et al. [2020], the Belousov-Zhabotinsky reaction, and Conway's Game of Life. These systems are selected for their diverse dynamics to assess the capability of NCA models to generalise beyond the generation of static patterns to dynamic systems. We study how carefully curated training regimes can induce desired behaviours such as long-term stability and structural recovery, and reveal the critical role the hidden channels play in guiding the behaviour of the NCA model.

Inferring the Rules

To allow the model to learn to exhibit long-term dynamics, we introduce a multi-step training regime.

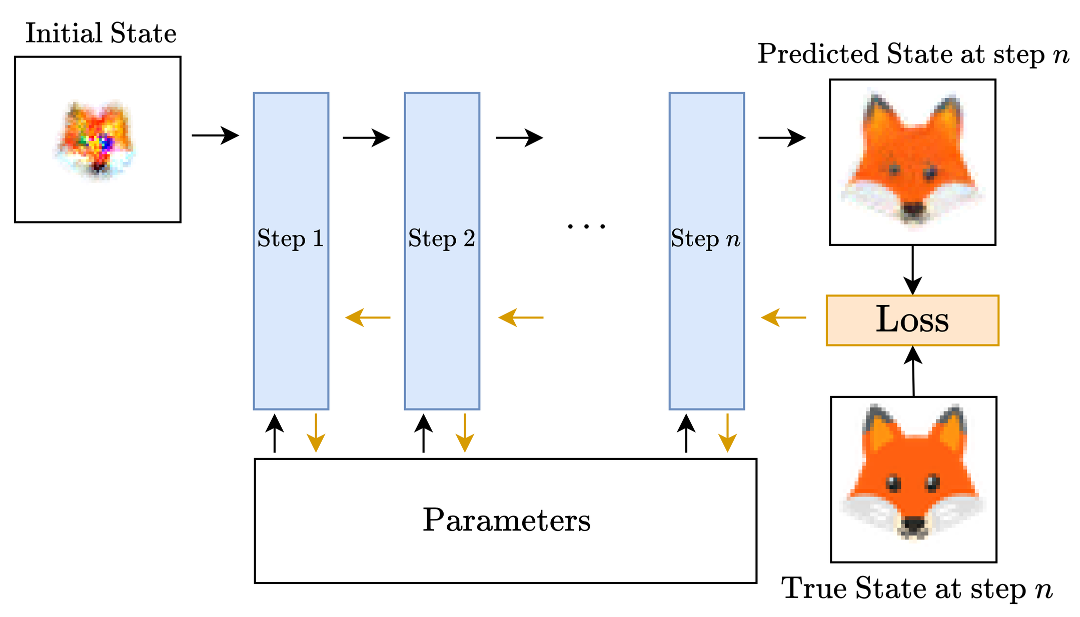

Figure 1. Schematic of the multi-step training strategy.

We find that stratified sampling from the different phases of the system evolution, with an emphasis on the growing phase, ensures that the NCA model is able to accurately replicate the dynamics of the target system. This strategy is also effective at teaching the NCA to replicate the behaviour of Conway's Game of Life and the BZ reaction, demonstrating the ability of NCA models to replicate the behaviour of diverse systems, provided that the training regime is adapted to the system.

Influence of Hidden Channels

We explore how the hidden channels of the model control the behaviour of the morphogenesis system of Mordvintsev et al. [2020]. During the growth phase, all channels are active in the pattern. However, in the stable phase, different channels are active in different physical locations of the pattern, using the channels to encode the final pattern.

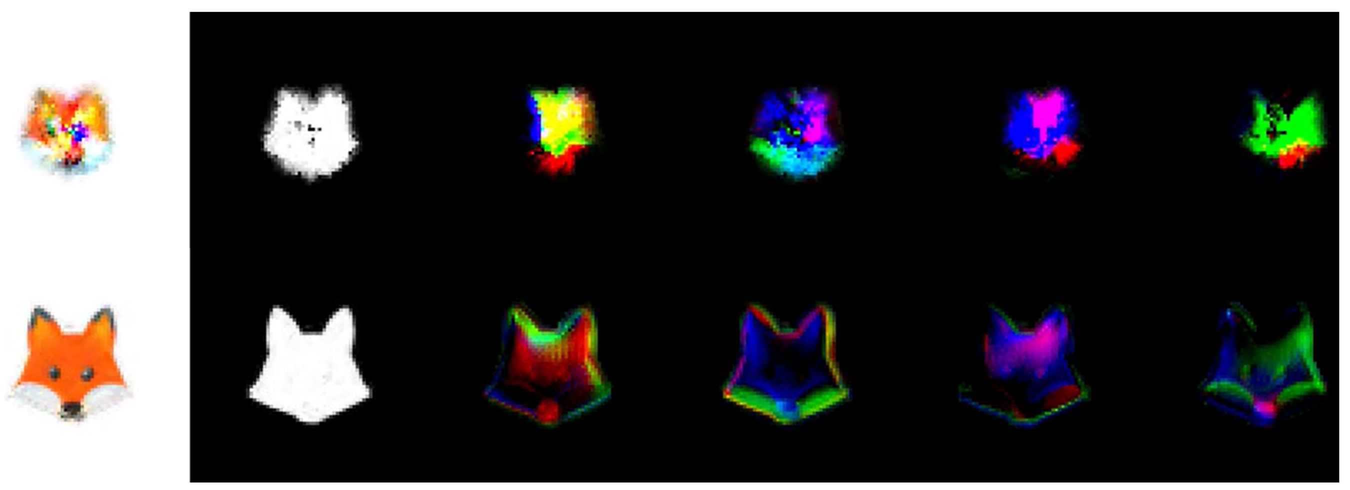

Figure 2. Snapshot of the morphogenesis model displaying all 16 channels at the growing (top) and stable (bottom) phases. The first column displays the RGB channels, the second column displays which cells are alive, and the four other columns display three of the hidden channels each.

The spatial location of cells is encoded in the hidden channels, allowing the different features of the pattern to be grown at different locations despite using a common update rule for all the cells. Figure 2 shows a visualisation of the channels for when the system is in the growing and stable phases. When the system is still growing, the expression of all the channels is still changing for each cell, and there is overlap between the locations where each channel takes a high value. However, in the stable state the cells differentiate themselves, using different channels to encode information about their role within the pattern.

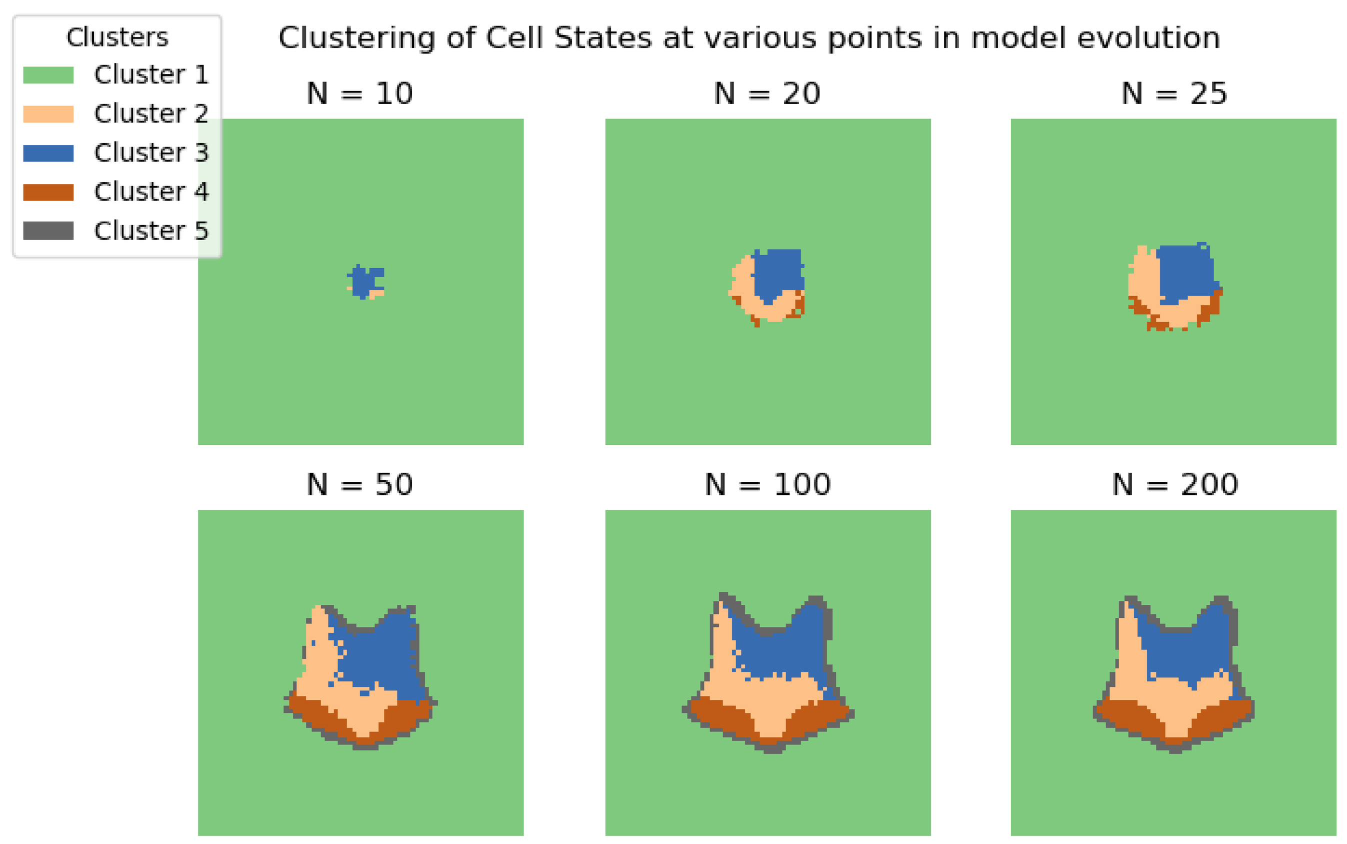

Figure 3. Visualisation of clustering of the cells of different stages in the evolution of the system into five clusters.

The insight that the system uses the hidden channels to encode spatial information helps explain previous results, which show that reducing the number of channels available to an NCA model diminishes its ability to perform the task of image morphing [Richardson et al., 2024].

Conclusions

Our study reaffirms the ability of neural cellular automata to replicate complex, emergent behaviour through localised interactions. By designing training strategies that emphasise different phases of morphogenetic evolution, growth, stability, and regeneration, we demonstrate that NCAs can internalise sophisticated rule-based behaviours from data alone, demonstrating their great potential to model arbitrary dynamics.

We further highlight the critical role of hidden channels in modulating emergent behaviours, suggesting that these internal representations function analogously to latent fields in biological development. Our experiments show that NCAs not only reconstruct known dynamics but can also generalise to novel behaviours such as pattern reproduction, hinting at their broader applicability in artificial life.

Future Directions

As neural CA continue to blur the boundaries between rule-based simulation and learned behaviour, future work should explore their use in a wider variety of domains, from agent-based modelling to distributed computing, and investigate the extent to which they can discover interpretable representations of the emergent systems they emulate.

References

Alexander Mordvintsev, Ettore Randazzo, Eyvind Niklasson, and Michael Levin. Growing neural cellular automata. *Distill*, 2020. doi: 10.23915/distill.00023. URL `https://distill.pub/2020/growing-ca`.

Alex D. Richardson, Tibor Antal, Richard A. Blythe, and Linus J. Schumacher. Learning spatio-temporal patterns with neural cellular automata. *PLOS Computational Biology*, 20(4):1–27, 04 2024. doi: 10.1371/journal.pcbi.1011589. URL `https://doi.org/10.1371/journal.pcbi.1011589`.

Acknowledgements

We thank the Accelerate Programme for Scientific Discovery for funding this work.

Code for this work is available under the MIT license at `https://github.com/archonus/nca_inference`