Investigating dynamics of Neural Cellular Automata in complex systems

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Abstract

Neural cellular automata (NCA) provide a powerful computational paradigm for modelling morphogenetic processes through local interactions and self-organization. We apply NCAs to a number of prototypical complex systems ranging from morphogenesis to reaction-diffusion systems. We explore the capacity of NCA to not only replicate complex visual patterns, but also to learn the underlying update rules of dynamic systems from spatiotemporal snapshots. We reproduce the behaviour of a morphogenesis system through various training regimes and demonstrate how training strategies critically influence the ability of the NCA to grow, persist, and regenerate patterns. 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 generalize 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.

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Introduction

Cellular automata have long served as a compelling framework for studying complex systems through simple local rules. Recent work by Mordvintsev et al. (2020) introduced a neural formulation of cellular automata (NCA) that combines traditional automata with neural networks. This approach encodes the state of each cell in multiple channels and evolves the system through convolutional update rules. The original NCA model demonstrated an impressive capability to self-organise and regenerate patterns. However, it remains an open question whether such systems can generalise and be used to infer rules underlying arbitrary spatiotemporal phenomena.

In this paper, we explore the potential of NCA to learn the dynamics of a system from observation alone. We study how carefully curated training regimes can induce desired behaviours such as long-term stability and structural recovery. 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.

Inferring the Rules

We investigate whether neural cellular automata can be used to reproduce complex behaviour by inferring the rules of a system given only snapshots of how the system evolves. The first training regime used was to simply provide the model with a snapshot given as input and its successor as the target, so that the model would learn the update rule. However, we found that although the model was quite accurate when predicting a single step, it failed to learn the long-term dynamics of the system, displaying instability over longer periods.

To allow the model to learn to exhibit long-term dynamics, the loss must be computed over multiple steps. The multi-step training regime randomly chooses a number n and computes the loss between the model prediction of the state n steps into the future and the true state of the frame at that time step. This training regime is much more effective than the single-step regime, exhibiting the correct growth and stability behaviour; however, the model still suffered from the fact that the growth stage in the training data was relatively small, which meant that the model was not able to reproduce the pattern to the level of detail of the original.

The behaviour of the morphogenesis system can be broadly categorised into two parts: the growing stage, where the seed grows into the pattern over successive updates, and the stable stage, where once the target pattern has been created, successive updates do not change the pattern. The state of the system is controlled by the hidden channels. A middle ground is when the system is regenerating a pattern: here, the system maintains the persistence behaviour for most of the image, but exhibits growth on the damaged section. In order to ensure that the NCA we trained also exhibited this behaviour, multiple runs of the model were used as training data: one where the system is growing, one where the system is stable, and one where the system is regenerating. Stratified sampling from each of these phases was used per batch, with an emphasis on the growing phase. This ensures that the model does not just learn the simpler behaviour of persisting an already grown image, but is also able to grow it from scratch like the original morphogenesis system. A similar strategy is effective at teaching the NCA to replicate the behaviour of Conway's Game of Life and the Belousov–Zhabotinsky reaction.

Influence of Hidden Channels

The hidden channels of the model are crucial to controlling the behaviour of the morphogenesis system. Although the morphogenesis model is only directly trained by taking the L2 loss over the RGBA channels, the hidden channels govern the behaviour of the model. 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.

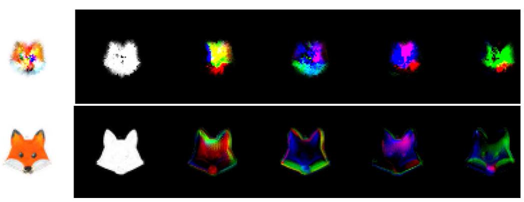

Figure 1: Snapshot of the morphogenesis model displaying all 16 channels at the growing (top) and stable (bottom) phases. The first image is the RGB channels, the second image is of the alpha channel which is used to determine whether a cell is considered alive or dead, and the four other images display three of the hidden channels each.

A key finding of this work is insight into how information about 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 1 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.

To analyse the spatial distribution of cells with similar states, clustering is performed on the cell states. The k-means clustering algorithm was applied to cluster the cell states, visualised in Figure 2. During the growing stage, the cells are all similar, however as the system grows, the cells differentiate and specialise. The cells which form the boundary all belong to the same cluster, suggesting that the boundary cells encode that information in the hidden channels to regulate the growth of the pattern. This insight into the behaviour of the morphogenesis system 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). Using fewer channels limits the model's capacity to encode information about the pattern features, thereby affecting the model's ability to produce detailed patterns and exhibit complex behaviour.

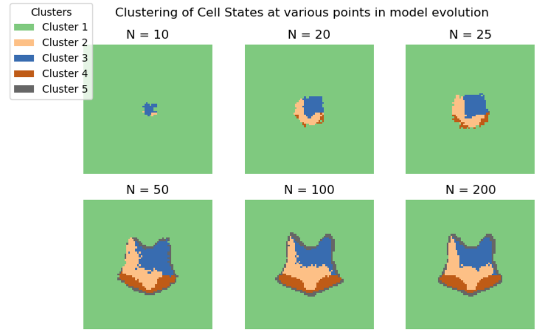

Figure 2: Visualisation of clustering of the cells of the stable state of the system into five clusters.

Conclusion

Our study reaffirms the ability of neural cellular automata to replicate, persist, and regenerate complex patterns 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. The stratified multi-step training regime proves especially effective in balancing these phases and in preventing models from degenerating into trivial persistence or overfitting to short-term 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. As neural CA continue to blur the boundaries between rule-based simulation and learned behaviour, future work should explore their use in more abstract domains, from agent-based modelling to distributed computation, and investigate the extent to which they can discover interpretable representations of the systems they emulate.

References

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