Learning Graph Cellular Automata

Anonymous Author(s)
Affiliation
Address
email

Abstract

Cellular automata (CA) are a class of computational models that exhibit rich dynamics emerging from the local interaction of cells arranged in a regular lattice. In this work we focus on a generalised version of typical CA, called *graph* cellular automata (GCA), in which the lattice structure is replaced by an arbitrary graph. In particular, we extend previous work that used convolutional neural networks to learn the transition rule of conventional CA, and we use graph neural networks to learn a variety of transition rules for GCA. First, we present a general-purpose architecture for learning GCA, and we show that it can represent any arbitrary GCA with finite and discrete state space. Then, we test our approach on three different tasks: 1) learning the transition rule of a GCA on a Voronoi tessellation; 2) imitating the behaviour of a group of flocking agents; 3) learning a rule that converges to a desired target state.

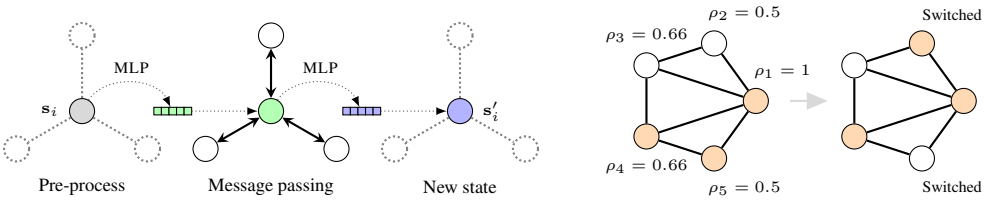
1 Introduction

Cellular automata (CA) [1] are discrete computational models that consist of a regular lattice of cells, each associated with a state, and a transition rule. The transition rule is usually defined to update the state of each cell as a function of its current state and the state of its neighbours. Even when using simple transition rules and low-dimensional lattices, CA can exhibit very intricate patterns that emerge from the repeated synchronous application of the transition rule. Despite being almost a century-old idea, many different forms of CA are still studied today in dynamical systems theory [2]. In this paper, we focus on a generalised version of CA called *graph cellular automata* (GCA) [3], which relaxes the assumption of the lattice structure and allows cells to have an arbitrary and variable number of neighbours.

Starting from the observation that GCA are a generalised version of lattice-based CA, in which the underlying lattice is replaced by an arbitrary graph, we focus on the analogous parallel that exists between convolutional neural networks (CNNs) and graph neural networks (GNNs) [4, 5, 6]. Namely, the goal of this paper is to study the application of GNNs to learn a desired GCA transition rule, a setting that we refer to as *Graph Neural Cellular Automata* (GNCA).

The inspiration for this work comes from a recent series of papers that studied how to train a convolutional neural network to approximate a desired CA transition rule, which we extend in two significant ways. First, we present a general-purpose architecture for GNCA and show that it is sufficient to represent any arbitrary GCA with finite and discrete state space. Based on well-known results on the expressive power of neural networks and GNNs, we also propose that the same architecture is expressive enough to represent any transition function on continuous state spaces. Then, we present several classes of problems that can be formulated as computation with GCA. We use our architecture to learn a varied family of GCA with non-trivial features including discrete and continuous state spaces, complex or unknown transition rules, dynamic graphs, and the ability to globally coordinate through local message exchanges. First, we train a GNCA to approximate a GCA defined on the Voronoi tessellation of random points, where the underlying graph is fixed throughout

Submitted to 35th Conference on Neural Information Processing Systems (NeurIPS 2021). Do not distribute.



(a) Schematic view of GNCA computation.

(b) Voronoi GCA transition.

Figure 1: (a) Schematic view of the GNCA computation. The central block represents the message-passing function of Eq. (4). (b) Example transition of a Voronoi GCA with binary states (represented by colours) and transition rule as described in Eq. (5) with $\kappa = 0.6$. Cells with a neighbourhood density $\rho_i < \kappa$ switch state.

the evolution of the system and the state space is binary. Then, we focus on a dynamic GCA with continuous state space and variable connectivity between cells. We consider the Boids algorithm [7], a Markovian and distributed multi-agent system designed to simulate the flocking of birds, and we train the GNCA to reproduce its behaviour. Finally, we consider the task of learning GNCA that converge to a target state in a continuous state space. Specifically, we train the GNCA to reconstruct the coordinates of a geometric point cloud.

The practical implications of this work are evident when considering that distributed systems are 1) the norm in nature, where complex behaviour is observed as an emergent property of simple and distributed computation, and 2) ubiquitous in technology, with the advent of cyber-physical systems that need to operate and react to local events while coordinating to achieve a target behaviour (for example, self-driving cars that act locally to avoid crashes but must prevent traffic globally). By applying GNNs to model GCA on systems described by graphs, we enable the discovery of unknown rules that allow us to solve tasks through emergent and distributed computation.

2 Related works

This work extends the results of many foundational works on learning CA with neural networks, which so far have only focused on regular lattices.

One of the first seminal works to draw a parallel between CA and neural networks was that of Gilpin [8], in which the author showed how to implement the transition rule of a CA using the receptive field of a CNN, as well as showing that any arbitrary binary rule could also be learned end-to-end with gradient descent.

Following up on the analysis of how CNNs can learn CA, Springer and Kenyon [9] observed that CNNs often fail to converge to exact solutions when trained to reproduce the Game of Life ruleset and that they often require many more parameters than the minimal number necessary to implement the exact transition rule, as predicted by the lottery ticket hypothesis [10]. The idea of learning 2D CA transition rules was also explored by Aach et al. [11], who proposed an encoder-decoder architecture with the ability to generalise to unseen neighbourhood configurations and sizes.

Mordvintsev et al. [12] recently introduced Neural Cellular Automata (NCA). The idea of NCA is to use a convolutional neural network to learn the transition rule of a 2D CA with a continuous and multi-dimensional state space, which they interpret as an image. In particular, they trained the NCA to converge to a specific image. They showed that, with proper training, NCA could reconstruct missing patches of the target image and were resilient to many classes of state perturbations. Randazzo et al. [13] extended their previous work on NCA by showing that neural cellular automata could be used to classify MNIST digits. This is an example of local behaviour leading to a global agreement about the overall structure of the system.

Since a CNN can be interpreted as a particular case of a GNN with fixed-size neighbourhood and anisotropic filters, what we propose here is a general extension of the works mentioned above.

3 Method

3.1 Graph Cellular Automata

A GCA is a 4-tuple $(\mathcal{G}, \mathcal{S}, \mathcal{N}, \tau)$ where $\mathcal{G} = (V, E)$ is a graph with node set V ($|V| = n$) and edge set $E \in V \times V$, $\mathcal{S}$ is the state set, $\mathcal{N} : V \to 2^V$ is the neighbourhood function s.t. $\mathcal{N}(i) = \{j \mid (j, i) \in E\}$, and $\tau : \mathcal{S} \to \mathcal{S}$ is a local transition rule. Let $\mathbf{s}_i \in \mathcal{S}$ indicate the state of node i. The transition rule is then defined as

$$\tau(\mathbf{s}_i) : \{\mathbf{s}_i\} \cup \{\mathbf{s}_j \mid j \in \mathcal{N}(i)\} \mapsto \mathbf{s}'_i. \tag{1}$$

For brevity, we denote with $\mathbf{S} \in \mathcal{S}^n$ the state configuration for the entire automaton and we write $\mathbf{S}' = \tau(\mathbf{S})$ to indicate the synchronous application of τ to all cells.

The original CA formalism allows for transition rules that can treat the different neighbours of a cell differently, according to their position with respect to the cell. This idea is, for instance, at the base of the Wolfram code for enumerating CA transition rules [14]. In GCA a similar anisotropic behaviour can be obtained by uniquely enumerating the neighbours of each cell and adapting the transition rule accordingly. More generally, we can assign to each edge $(i, j) \in E$ an attribute $\mathbf{e}_{ij} \in \mathbb{R}^{d_e}$ encoding, for example, the direction, distance, or angle of node i relative to node j. It is also possible to consider any arbitrary attributes associated with edges, representing abstract relations between any two neighbouring cells. In short, we can see anisotropy in GCA as a dependence of the transition rule on the specific relation that exists between a cell and a neighbour:

$$\tau(\mathbf{s}_i) : \{\mathbf{s}_i\} \cup \{\mathbf{s}_j, \mathbf{e}_{ji} \mid j \in \mathcal{N}(i)\} \mapsto \mathbf{s}'_i. \tag{2}$$

The usefulness of this definition will become evident in later sections.

3.2 Graph Neural Networks

Graph Neural Networks (GNNs) are a family of models designed to process graph-structured data. The core functionality of many GNNs can be described with a message-passing scheme. Let $\mathbf{h}_i \in \mathbb{R}^{d_h}$ represent a vector attribute associated with the ith node of a graph and $\mathbf{e}_{ij} \in \mathbb{R}^{d_e}$ an edge attribute as defined above. A message-passing GNN is a function that computes a vector $\mathbf{h}'_i \in \mathbb{R}^{d'_h}$ according to the following scheme:

$$\mathbf{h}'_i = \gamma\left(\mathbf{h}_i, \square_{j \in \mathcal{N}(i)}\, \phi\left(\mathbf{h}_i, \mathbf{h}_j, \mathbf{e}_{ji}\right)\right), \tag{3}$$

where ϕ is the message function, $\square$ is a permutation-invariant operation to aggregate the set of incoming messages, and γ is the update function. When ϕ, $\square$, and γ are differentiable operations, message-passing layers can be stacked and their parameters can be learned end-to-end with backpropagation and stochastic gradient descent.

In this work, specifically, we adopt a message-passing architecture inspired by You et al. [15] s.t.

$$\mathbf{h}'_i = \mathbf{h}_i \,\Big\|\, \sum_{j \in \mathcal{N}(i)} \text{ReLU}(\mathbf{W}\mathbf{h}_j + \mathbf{b}), \tag{4}$$

where $\|$ indicates vector concatenation, ReLU is the Rectified Linear Unit activation, and $\mathbf{W} \in \mathbb{R}^{d'_h \times d_h}$ and $\mathbf{b} \in \mathbb{R}^{d'_h}$ are trainable parameters. The message-passing block is also preceded and followed by multi-layer perceptrons (MLPs) with ReLU activations, whose task is to learn non-relational transformations of the node features [15]. The architecture is schematically shown in Fig. 1a. Note that Eq. (4) can easily be extended to account for edge attributes as well, although we will see in later sections that different use cases may benefit from different ways of incorporating that information. We mention two main techniques to achieve this kind of anisotropy, both based on making the message function ϕ edge-dependent: 1) the weights matrix $\mathbf{W}$ can be computed as a function of $\mathbf{e}_{ji}$, through a *kernel generating network* [16], and 2) $\mathbf{e}_{ji}$ can be concatenated to $\mathbf{h}_j$ to compute the messages.

3.3 Graph Neural Cellular Automata

The goal of this paper is to explore the parallel that exists between GCA and GNNs. In particular, here we consider a setting in which the state transition function of a generic GCA is approximated with a GNN, which we indicate as a *Graph Neural Cellular Automaton* (GNCA).

The relation between the two models can be immediately seen by comparing Equations (2) and (3), as the GNN model contains all the necessary elements to describe a GCA transition rule. First, when the GNN is configured so that $d_h = d'_h$, then both functions are endomorphisms that depend only on node i and its neighbourhood $\mathcal{N}(i)$. Then, by considering $\mathcal{S} \equiv \mathbb{R}^{d_h}$, the state of the GCA can be interpreted as a graph signal s.t. $\mathbf{h}_i = \mathbf{s}_i$. Finally, as previously mentioned, the GNN can be configured to take into account edge attributes, allowing it to model transition rules that can be both isotropic or anisotropic.

We indicate with $\tau(\mathbf{S})$ the transition function of a GCA and with $\tau_\theta(\mathbf{S})$ the transition function of a GNCA with learnable parameters θ. The dependency of either function on graph $\mathcal{G}$ is left implicit. Finally, we use d to indicate the states' dimension. The specific GNN architecture of τ_θ that we consider in Eq. (4), besides being motivated by the results of You et al. [15], has a sufficiently high number of parameters which, as noted by Springer and Kenyon [9], can be a deciding factor for learning the transition rule of a CA. This requirement is also somewhat reflected by the architectural choices of Mordvintsev et al. [12].

Implementing GCA with M-state space One of the main results of Gilpin [8] was to show different ways to implement an arbitrary M-state CA with a CNN. The most straightforward implementation proposed by the author relied on two main neural computation blocks:

1. Two convolutional layers with 1x1 filters, to compute a one-hot encoding of the states;
2. One convolutional layer with 3x3 filters, to match all of the possible input patterns of the transition rule and compute the corresponding output.

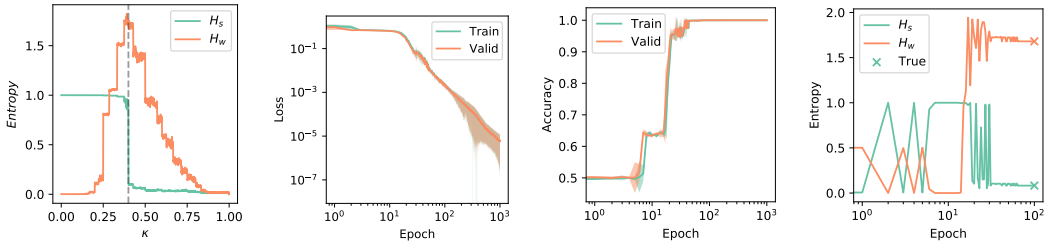
The general principle used to design the transition rule of a CA with a CNN can be straightforwardly extended to GCA and GNNs. Consider a GCA with state space $\mathcal{S} = \{1, ..., M\}$ and n cells, with maximum node degree $d_{max} \leq n$ (and, usually, $d_{max} \ll n$).

The first block of Gilpin's implementation remains the same, since it is a transformation applied only to each individual node, independently of its neighbours. The second block requires us to be more careful. First, we note that Gilpin's implementation covers the most general case in which the transition rule is anisotropic. By generalising this principle to the case of GCA, as discussed in Sec. 3.1, we require that each cell has up to d_{max} neighbours identified by a unique one-hot vector edge attribute of size d_{max}. The pattern matching mechanism proposed by Gilpin can then be implemented with a bank of d_{max} weight matrices of shape $M \times M^{d_{max}}$, that is used to compute the message from each neighbour, according to its associated edge attribute (*e.g.*, consider the work of Simonovsky and Komodakis [16]).

We note, however, that this case represents an upper bound in complexity, since many GCA rely on isotropic rules and better implementations can be obtained if the structure of the GCA rule is known. For example, Conway's Game of Life can be implemented with a CNN consisting of one convolutional layer with 3x3x5 filters, with one channel to implement the identity and four channels to count neighbours, and two convolutional layers with 1x1x5 filters for pattern-matching [8]. We note that the GNCA covers this result as it natively implements the identity (the concatenation of Eq. (4) can be replaced with a sum to match the exact implementation) and neighbour counting can be achieved with $\mathbf{W} = [1, 1, 1, 1]$ and $\mathbf{b} = [-1, -2, -3, -4]$ (*cf.* [8, Appendix A]). Finally, the 1x1x5 convolutional layers are equivalent to the post-processing dense layers described in Sec. 3.2.

In Sec. 4.1, we will see a similar minimal implementation for an outer-totalistic GCA.

Extension to continuous state space We can also conjecture that the architecture described in Sec. 3.2 is expressive enough to represent any transition function for a GCA with continuous state space. First, it is a well-known result of machine learning theory that a two-layer MLP is, when appropriately configured with a sufficient number of neurons, a universal approximator for any Borel measurable function. The pre-processing MLP of the general GNCA architecture is therefore sufficient to compute any desired representation of the states. Then, building on the results of Zaheer et al. [17], we can also see that the structure of the GNCA allows us to model any permutation invariant function of the neighbours. Finally, by concatenating the representation of a node to the representation of its neighbours and giving the result as input to the post-processing MLP, we are also able to compute any transition to the following state. Of course, these results are conditioned on



(a) Entropy vs. κ. (b) Loss. (c) Accuracy. (d) Entropies vs. training.

Figure 2: (a) Shannon H_s and word H_w entropy vs. threshold κ for the Voronoi GCA. The edge-of-chaos transition is marked at $\kappa = 0.4$. (b) Median training and validation loss of the GNCA. (c) Median training and validation accuracy of the GNCA.[1](d) Entropy of the GNCA as training progresses. The two "x" indicate the real entropy values of the target Voronoi GCA.

the two MLPs being sufficiently large, and there are no guarantees that the training algorithm will be able to identify the correct function.

4 Experiments

We now consider different experiments aimed at showcasing the capabilities of our GCNA architecture. We take inspiration from the literature on learning lattice-based CA to design three experimental settings with different goals. First, we show a basic application to confirm that the GNCA is indeed capable to learn a desired GCA transition rule via supervised learning. Then, we extend this setting to a more complex case in which the state space is continuous and the underlying graph is dynamic, to demonstrate the applicability of the GNCA to multi-agent systems modelling. Finally, we consider the task of learning an unknown transition rule simply by specifying the target behaviour of the GNCA. Specifically, we extend the work of Mordvintsev et al. [12] to the GCA case and train our GNCA to converge to a desired state. Here we report a summary of the experiments and refer the reader to the supplementary material for more details.

4.1 GNCA on Voronoi tasselation

We begin by studying a binary GCA with density-based transition rules and threshold dynamics [18], and for which $\mathcal{G}$ is given by the Delaunay triangulation of a random 2D point cloud. The cells of this type of GCA are the cells of the Voronoi tessellation of the points. Let $\mathcal{S} = \{0, 1\}$ be a binary state space, $\rho_i = \frac{1}{|\mathcal{N}(i)|} \sum_{j \in \mathcal{N}(i)} \mathbf{s}_j$ the neighbourhood density of a node, and $\kappa \in [0, 1]$ a threshold, then the GCA rule is given by:

$$\tau(\mathbf{s}_i) = \begin{cases} \mathbf{s}_i, & \text{if } \rho_i \geq \kappa \\ 1 - \mathbf{s}_i, & \text{if } \rho_i < \kappa \end{cases}. \tag{5}$$

An example transition on such a *Voronoi GCA* is shown in Fig. 1b.

The goal of this experiment is to study the base case in which $\mathcal{G}$ is static and planar, which is the simplest extension of typical outer-totalistic CA (like the Game of Life) to the setting of an irregular arrangement of the cells. Having a binary state space simplifies the problem and allows us to treat this as a node classification task.

Measures of GCA complexity Following the method of Marr and Hütt [18], we quantify the complexity of our finite-state GCA using two entropy measures, estimated from the sequences of states observed by repeatedly applying the transition rule. The average Shannon entropy is defined as $H_s = \frac{1}{n} \sum_{i=1}^{n} -p_i^s \log_2 p_i^s$, where p_i^s is the empirical probability that node i is in state s. The average word entropy is $H_w = \frac{1}{n} \sum_{i=1}^{n} (\sum_{l=1}^{t} -p_i^l \log_2 p_i^l)$, where p_i^l is the number of constant words of length l (for any state state) found in the state sequence of node i. When combined, these two

[1]For figures 2b and 2c, the curves have some significant outliers and therefore, instead of the mean and standard deviation, we report the median and the median absolute standard deviation interval over 5 runs.

measures are informative enough to separate GCA into the four Wolfram classes of CA complexity [18]. As shown in Fig. 2a, the Voronoi GCA considered here has a sharp edge-of-chaos transition at around $\kappa = 0.4$, above which the CA switches to non-chaotic dynamics. This is marked by a sharp decrease in Shannon entropy and by reaching peak word entropy (which indicates the occurrence of interesting patterns of states). In the following experiments, we consider $\kappa = 0.42$ as it exhibits both non-chaotic and non-trivial dynamics.

Training We start by computing $\mathcal{G}$ as the Delaunay triangulation of $n = 1000$ random points sampled uniformly in $[0, 1] \times [0, 1]$. We generate training examples for the model by sampling mini-batches of random binary states $[\mathbf{S}^{(1)}, \ldots, \mathbf{S}^{(K)}]$, and we train the GNCA by minimizing the negative log-likelihood between the true successor states $\tau(\mathbf{S}^{(k)})$ and the predicted next states $\tau_\theta(\mathbf{S}^{(k)})$.

Results Figures 2b and 2c show the evolution of the GNCA's loss and accuracy on the training and validation sets, averaged over 10 runs. We see that the model quickly converges to a near-perfect approximation of the transition function and that the loss continues to gradually improve even after reaching 100% validation accuracy. Fig. 2d shows the Shannon and word entropies of the model as training progresses. To evaluate the entropy at each training epoch, the GNCA is evolved autonomously (*i.e.*, feeding its predictions back as input) for 1000 steps and the two entropy measures are computed from the observed state trajectories. Note that the GNCA's predictions are rounded to 0 or 1 during inference. This analysis lets us comment on two aspects. First, the GNCA is able to quickly learn a transition function with a very similar entropy to the true transition function (marked with an "x" in the figure), although it takes a while to reach the exact target values. Second, we see that the GNCA eventually learns a robust approximation of the true transition function, which does not diverge from the true trajectory when evolved autonomously.

Minimal exact implementation As discussed in Sec. 3.3, when the form of the transition rule is known, it is often possible to provide a much more compact implementation of the GNCA. For the rule described in Eq. (5), we can see that the GNCA has to implement (or learn to implement) two main operations: calculating the density of alive neighbours and mapping the state to its successor as a function of the state itself, the density, and the threshold κ. The first step can be achieved with a minor modification to Eq. (4) to use an average aggregation instead of the sum, and by setting $\mathbf{W} = 1$ and $\mathbf{b} = 0$. Alternatively, it is also possible to keep the sum aggregation and set $\mathbf{W} = [1, 0]$, $\mathbf{b} = [0, 1]$ (one neuron to count alive neighbours, and one to count all neighbours), although this requires an extra neuron in the following block. We also remove the pre-processing MLP since the states themselves are enough to compute the required representation. Then, the transition can be computed with the post-processing MLP of the GNCA. As shown in Fig. 3, we see that the transition rule of Eq. (5) is essentially equivalent to the famous XOR problem [19, 20] and can therefore be solved with a MLP with 2 hidden neurons and one output neuron. We empirically trained one such architecture with ReLU hidden activation and sigmoid output (mimicking the structure of the full post-processing MLP described above) and found that one possible solution is given by the following set of weights:

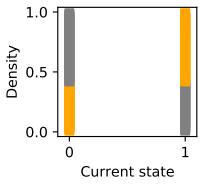
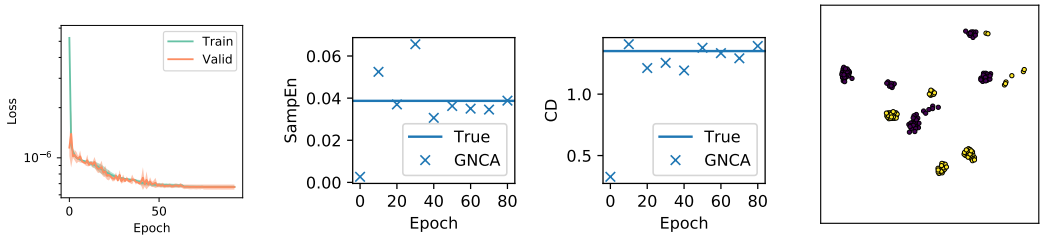


Figure 3: GCA rule of Eq. (5). Colours indicate the output: grey is 0, orange is 1.

$$\mathbf{W}_1 = \begin{bmatrix} -1.98 & 1.64 \\ 2.63 & -2.8 \end{bmatrix}; \quad \mathbf{b}_1 = [-0.46 \quad 0.17]; \quad \mathbf{W}_2 = [-3.3 \quad -3.3]; \quad \mathbf{b}_2 = [2.1].$$

4.2 GNCA for agent-based modeling

Our second experiment consists of learning a GCA with continuous state space and in which the connectivity between cells changes over time. Specifically, we take a set of cells whose states represent their positions and velocities on a plane, $\mathcal{G}$ is a dynamic graph given by a fixed-radius neighbourhood of each cell at each step, and the state of the cells is updated with the Boids algorithm [7]. This setting is more general than the previous two experiments, since $\mathcal{G}$ is now a dynamic graph, and possibly a more realistic approximation of many real-world phenomena. We still consider this as a kind of CA since the characterising feature of CA is that the transition function depends on a cell's neighbours and is Markovian, although this setting is better described as a generic multi-agent system.



(a) Loss. (b) SampEn and CD vs. training epoch. (c) Examples of flocks.

Figure 4: (a) Average and standard deviation of the training and validation loss of the GNCA (5 runs). (b) SampEn and CD of the GNCA as training progresses. The horizontal lines indicate the true values of the target boids GCA. (c) Examples of flocks forming in the true boids system (purple) and the learned GNCA (yellow).

The transition function of the Boids algorithm is highly non-linear and is summarised in Algorithm 1. Briefly, at each step, the velocity of each boid is updated and its position changes accordingly. The new velocity of each boid is computed as a function of its current velocity and the positions and velocities of the neighbours. Finally, some constraints on the maximum speed and turn angle are enforced, as well as a soft-boundary condition that pushes the boids away from the edges of the simulation box.

Algorithm 1: Pseudo-code for Boids [7].

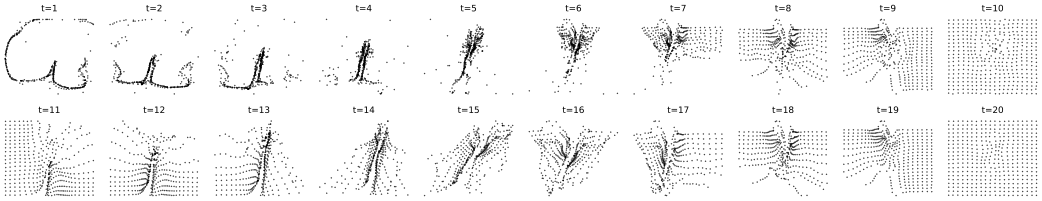
Input: n: n. of boids; T: n. of steps;
for $i \leftarrow 1$ **to** n **do**
  Initialise random $\mathbf{p}_i, \mathbf{v}_i \in \mathbb{R}^2$
end
for $t \leftarrow 1$ **to** T **do**
  Compute neighbours
  for $i \leftarrow 1$ **to** n **do**
    if $\mathbf{p}_i$ *is close to boundary* **then**
      $\mathbf{a}_b \leftarrow$ Steer away from boundary
    end
    $\mathbf{a}_s \leftarrow$ Avoid collisions with neigh.
    $\mathbf{a}_a \leftarrow$ Align to velocity of neigh.
    $\mathbf{a}_c \leftarrow$ Align to position of neigh.
    $\mathbf{a}_i \leftarrow \mathbf{a}_b + \mathbf{a}_s + \mathbf{a}_a + \mathbf{a}_c$
    $\mathbf{v}_i \leftarrow \mathbf{v}_i + \mathbf{a}_i$
    $\mathbf{v}_i \leftarrow$ Enforce speed and turn limits
    $\mathbf{p}_i \leftarrow \mathbf{p}_i + \mathbf{v}_i$
  end
end

Training To train the GNCA we generate trajectories by letting 100 boids evolve for 500 timesteps, starting from randomly initialised positions and velocities. We generate 300 trajectories for training, 30 for validation and early stopping, and 30 for testing the final performance of the GNCA. The model is trained, like in the previous case, to approximate the true transition $\tau(\mathbf{S})$.

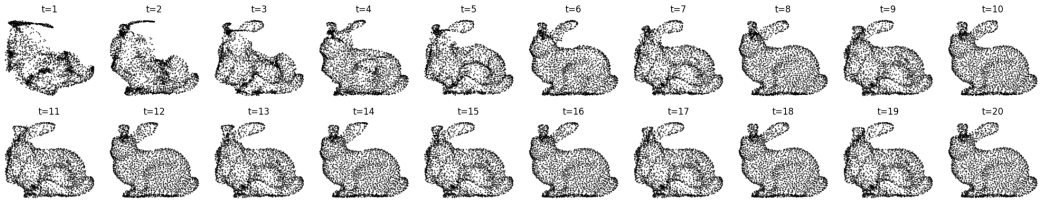
Table 1: Complexity measures for the true Boids system and the trained GNCA.

	SampEn	**Corr. dim.**
True	0.0369 $\pm$ 0.0053	1.3125 $\pm$ 0.1444
GNCA	0.0302 $\pm$ 0.0079	1.3017 $\pm$ 0.1336

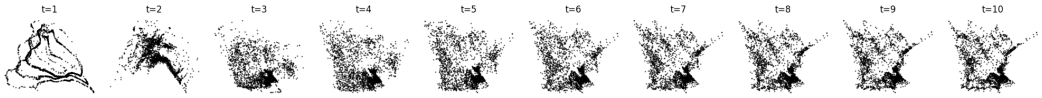
Results One key aspect of approximating a continuous-state GCA is that errors in the prediction will quickly accumulate, making it almost impossible for the GNCA to perfectly imitate the true system. For this reason, despite quickly reaching a training, validation, and test error in the order of 10^{-7}, the GNCA cannot perfectly approximate the true trajectory of the target GCA when evolved autonomously. However, we can evaluate the quality of the learned transition function by using the sample entropy (SampEn) [21] and correlation dimension (CD) [22], two measures of complexity for real-valued time series. Table 1 compares the SampEn and CD of the true Boids system with the trained GNCA, computed from trajectories of 1000 steps and averaged over all boids and 5 random initialisations of the system. We see that both systems have very similar complexity measures, indicating that their behaviour is generating a comparable amount of information and is therefore similar. We report in Fig. 4b an example of how the SampEn and CD change as the GNCA is trained. Additionally, we see that the GNCA learns a flocking behaviour similar to the target system (shown in Fig. 4c), although with smoother and less precise trajectories. Notably, we observed that the GNCA has no trouble in learning the soft-boundary condition. We include videos of the GNCA trajectories as supplementary material.



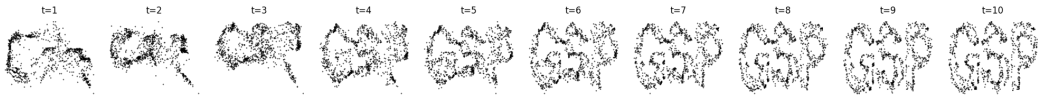
(a) Grid, trained with $t = 10$, example of limit cycle.



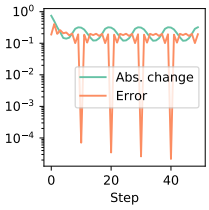
(b) Bunny, trained with $t = 10$, example of limit cycle.



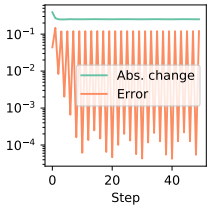
(c) Minnesota, trained with $t = 10$, example of convergence.



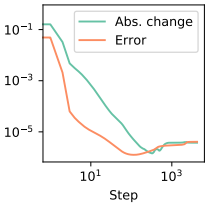
(d) Logo, trained with $t \in [10, 20]$, example of convergence.



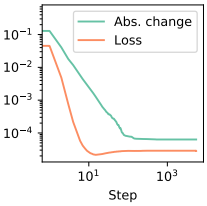
(e) Grid, $t = 10$.



(f) Bunny, $t = 10$.



(g) Minnesota, $t = 10$.



(h) Minnes., $t \in [10, 20]$.

Figure 5: Figs. (a), (b), (c): state trajectory of the trained GNCA on different graphs. Figs. (d), (e), (f), (g): loss and absolute change between consecutive states.

4.3 GNCA that converge to a fixed target

For our final experiment, we extend the previous work of Mordvintsev et al. [12] and study a setting in which a GNCA is trained to converge to a specific target state from a given initial condition. We consider several geometric graphs available in the PyGSP library [23], and we set the target state to be the 2D or 3D node coordinates, while $\mathcal{G}$ is kept fixed.

The goal of this experiment is twofold. First, we wish to study the setting in which the transition function that we are trying to approximate is unknown. Second, and more importantly, our goal is to show that the GNCA can learn local transition rules that result in a global coordination of the cells.

Training The main challenge in this experiment is to make the target state an attractor of the GNCA. In other words, let $\bar{\mathbf{S}}, \hat{\mathbf{S}} \in \mathbb{R}^d$ be the initial and target states, respectively, we wish to learn τ_θ s.t. $\tau_\theta^t(\bar{\mathbf{S}}) \to \hat{\mathbf{S}}$.[2]

[2]Here, we consider as initial state a normalisation of the target s.t. $\bar{\mathbf{s}}_i = \hat{\mathbf{s}}_i / \|\hat{\mathbf{s}}_i\|$.

To train the GNCA, we apply the transition for a given number of steps t and use backpropagation through time to update the weights, with loss $L = \frac{1}{K}\sum_{k=1}^{K}(\tau_\theta^t(\bar{\mathbf{S}}^{(k)}) - \hat{\mathbf{S}})^2$ for mini-batches of size K consisting of initial states $\bar{\mathbf{S}}^{(k)}$ for $k = 1, \ldots, K$. This ensures that the GNCA will learn to converge to the target state in t steps.

Second, during training, we use a cache to store the states $\tau_\theta^t(\mathbf{S})$ reached by the GNCA after each forward pass. Then, we use the cache as a replay memory and train the GNCA on batches of states $\bar{\mathbf{S}}^{(k)}$ sampled from the cache. For every batch, the cache is updated with the new states reached by the GNCA after t steps, and one element of the cache is replaced with $\bar{\mathbf{S}}$ to avoid catastrophic forgetting. The cache has a size of 1024 states and is initialised entirely with $\bar{\mathbf{S}}$. By using the cache, the GNCA is trained also on states that result from a repeated application of the transition function. This strategy encourages the GNCA to remain at the target state after reaching it, while also ensuring an adequate exploration of the state space during training.

Results We report in Fig. 5 the results obtained on the following graphs: a grid, the Stanford bunny geometric mesh, the Minnesota road network, the PyGSP logo, and a random point cloud sampled on the Swiss roll manifold. Figures 5a, 5b, and 5d show example trajectories of the trained GNCA for $t = 10$. We see that in all cases the model successfully learns to reach the target state in the prescribed number of steps, although it exhibits different behaviours for the subsequent steps. Figures 5e, 5f, and 5g show the mean squared error between the current state and the target as the trained GNCA is evolved. We see that, in the cases of the grid and bunny, the GNCA reaches a limit cycle and oscillates between states with a high loss and the target state (indicated by a very low loss). Alternatively, we see that for the Minnesota network the GNCA is able to reach a low-loss state in t steps, but then converges to a different state with higher loss. To improve convergence and make the target state more stable, one possibility is to train the GNCA with $t \in [10, 20]$ randomly sampled at each forward pass, as also done by Mordvintsev et al. [12]. The effect of this is shown in Fig. 5h for the Minnesota road network, for which the GNCA learns to remain at a stable state for $t > 10$ although the overall loss is higher. We observed the same pattern also for the other graphs, although the final loss at the stable state is much higher than the one reached in the limit-cycle attractor. We also note that the oscillating behaviour is likely due to using the state cache, since the backpropagation will only happen for states that have been computed for kt steps, for $k \in \mathbb{N}$. By sampling a random t at each forward pass, we can contrast this effect although this results in a loss of performance. Investigating reasons for this difference is left as future work.

5 Conclusions

We have studied the application of GNNs to implement the transition rule of GCA. We proposed a general-purpose architecture to achieve this, which we showed to be general enough to implement any arbitrary transition function for a large class of GCA. We have applied the GNCA model to learn a variety of GCA transition rules, including unknown rules for which we only specified a desired behaviour. We believe to have opened the way to a possible line of research in which GNNs can unlock the power of GCA and implement a desired behaviour through distributed and emergent computation.

References

[1] J. Neumann, A. W. Burks *et al.*, *Theory of self-reproducing automata*. University of Illinois press Urbana, 1966, vol. 1102024.

[2] K. Bhattacharjee, N. Naskar, S. Roy, and S. Das, "A survey of cellular automata: types, dynamics, non-uniformity and applications," *Natural Computing*, vol. 19, no. 2, pp. 433–461, 2020.

[3] C. Marr and M.-T. Hütt, "Outer-totalistic cellular automata on graphs," *Physics Letters A*, vol. 373, no. 5, pp. 546–549, 2009.

[4] M. Gori, G. Monfardini, and F. Scarselli, "A new model for learning in graph domains," in *Proceedings. 2005 IEEE International Joint Conference on Neural Networks, 2005.*, vol. 2. IEEE, 2005, pp. 729–734.

[5] F. Scarselli, M. Gori, A. C. Tsoi, M. Hagenbuchner, and G. Monfardini, "The graph neural network model," *IEEE Transactions on Neural Networks*, vol. 20, no. 1, pp. 61–80, 2009.

[6] P. W. Battaglia, J. B. Hamrick, V. Bapst, A. Sanchez-Gonzalez, V. Zambaldi, M. Malinowski, A. Tacchetti, D. Raposo, A. Santoro, R. Faulkner *et al.*, "Relational inductive biases, deep learning, and graph networks," *arXiv preprint arXiv:1806.01261*, 2018.

[7] C. W. Reynolds, "Flocks, herds and schools: A distributed behavioral model," in *Proceedings of the 14th annual conference on Computer graphics and interactive techniques*, 1987, pp. 25–34.

[8] W. Gilpin, "Cellular automata as convolutional neural networks," *Physical Review E*, vol. 100, no. 3, p. 032402, 2019.

[9] J. M. Springer and G. T. Kenyon, "It's hard for neural networks to learn the game of life," *arXiv preprint arXiv:2009.01398*, 2020.

[10] J. Frankle and M. Carbin, "The lottery ticket hypothesis: Finding sparse, trainable neural networks," *arXiv preprint arXiv:1803.03635*, 2018.

[11] M. Aach, J. Goebbert, and J. Jitsev, "Generalization over different cellular automata rules learned by a deep feed-forward neural network," *ArXiv*, vol. abs/2103.14886, 2021.

[12] A. Mordvintsev, E. Randazzo, E. Niklasson, and M. Levin, "Growing neural cellular automata," *Distill*, vol. 5, no. 2, p. e23, 2020.

[13] E. Randazzo, A. Mordvintsev, E. Niklasson, M. Levin, and S. Greydanus, "Self-classifying mnist digits," *Distill*, 2020, https://distill.pub/2020/selforg/mnist.

[14] S. Wolfram, "Statistical mechanics of cellular automata," *Reviews of modern physics*, vol. 55, no. 3, p. 601, 1983.

[15] J. You, R. Ying, and J. Leskovec, "Design space for graph neural networks," *arXiv preprint arXiv:2011.08843*, 2020.

[16] M. Simonovsky and N. Komodakis, "Dynamic edgeconditioned filters in convolutional neural networks on graphs," in *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, 2017.

[17] M. Zaheer, S. Kottur, S. Ravanbakhsh, B. Poczos, R. R. Salakhutdinov, and A. J. Smola, "Deep sets," in *Advances in neural information processing systems*, 2017, pp. 3391–3401.

[18] C. Marr and M.-T. Hütt, "Cellular automata on graphs: Topological properties of er graphs evolved towards low-entropy dynamics," *Entropy*, vol. 14, no. 6, pp. 993–1010, 2012.

[19] J. L. McClelland and D. E. Rumelhart, *Explorations in parallel distributed processing: A handbook of models, programs, and exercises*. MIT press, 1989.

[20] R. Bland, *Learning XOR: exploring the space of a classic problem*. Department of Computing Science and Mathematics, University of Stirling Stirling, 1998.

[21] J. S. Richman and J. R. Moorman, "Physiological time-series analysis using approximate entropy and sample entropy," *American Journal of Physiology-Heart and Circulatory Physiology*, 2000.

[22] P. Grassberger and I. Procaccia, "Characterization of strange attractors," *Physical review letters*, vol. 50, no. 5, p. 346, 1983.

[23] M. Defferrard, L. Martin, R. Pena, and N. Perraudin, "Pygsp: Graph signal processing in python." [Online]. Available: https://github.com/epfl-lts2/pygsp/

Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? **[TODO]**
   (c) Did you discuss any potential negative societal impacts of your work? [N/A]
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [N/A]
   (b) Did you include complete proofs of all theoretical results? [N/A]
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] Code is included in the supplementary material and available online (URL hidden for blind review).
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See supplementary material.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See supplementary material.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
   (b) Did you mention the license of the assets? [N/A]
   (c) Did you include any new assets either in the supplemental material or as a URL? [Yes] Code is included in the supplementary material and available online (URL hidden for blind review).
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]