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## Evolutionary Algorithms for the Discovery of Cellular Automata Transition Functions

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# **Abstract**

Evolutionary algorithms are effective tools for black-box optimisation problems.

## Acknowledgements

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# Chapter 1

## Introduction

### 1.1 Overview

Evolutionary algorithms (EAs) have long been held as effective tools for black-box optimisation problems. Grounded in the principles of Darwinian evolution, EAs traverse over a search space by performing selection, mutation, and crossover on a population of candidate solutions. Increasingly strong solutions are discovered as the fitness of the population grows.

Cellular automata (CAs) are discrete models of computation in which multiple "cells" are simultaneously updated at regular time steps such that the state of any cell depends exclusively on the state of the cells in a local neighbourhood around it in the previous time step. CAs are powerful computational engines due to their inherently parallel structure. However, they are more commonly utilised as an abstract representation to study nonlinear dynamics and the emergence of complexity.

Top-down investigations into CA behaviour are vast and varied. Mathematical analyses seek to taxonomize CA properties and prove general results about long-term behaviour from intrinsic properties. In the natural and social sciences, CAs are designed to model physical, biological, or human behaviour. Both of these endeavours seek to analyse the behaviour of a CA from its structure, transition function, and possibly initial conditions.

In this thesis, we explore a bottom-up approach where we deduce the underlying properties of a CA by observing its behaviour. In particular, we utilise EAs to search the rulespaces of several classes of CA. We tackle multiple optimisation problems from the imitation of particular CA behaviour to generation of desirable long-term states.

### 1.2 Objectives

We aim to develop a system to discover cellular automata that are highly likely to exhibit a desired behaviour.

### 1.3 Contributions

The key contributions of this project are as follows:

1. **Evolutionary Algorithm Toolkit**

A versatile toolkit that implements multiple evolutionary algorithms to train and optimise different classes of CA. We use this to successfully predict the update rule of binary outer-totalistic CA from observations of the CA running on random initial conditions. We show that this can be extended to continuous automata by predicting the parameters of diffusion-reaction equations from simulations of chemical reactions.



## 2. **Cellular Automaton Simulator**

A system that can efficiently simulate discrete and continuous cellular automata. This allows a broad range of fitness functions to be implemented in the EA toolkit. This can also render snapshots of the CA directly during simulation which allows animations to be efficiently generated afterwards.

## 3. **Procedural Maze Generator**

A CA-based maze generation program that uses the EA toolkit to produce difficult mazes with characteristics optimised to user preference.

# 1.4 Technical Challenges

## Chapter 2

# Preliminaries

### 2.1 Cellular Automata

A cellular automaton (CA) is a computational model that performs multiple parallel computations, each depending on local interactions, to produce complex global behaviour. We define a CA formally as follows.

**Definition 2.1** (Cellular automaton). *A cellular automaton is an  $n$ -dimensional finite grid of computational units called cells. Each cell  $c_i$  is characterised by:*

- A discrete state variable  $\sigma_i(t) \in \Sigma$ , where  $i$  indicates the index of the cell in the lattice,  $t$  indicates the current time step, and  $\Sigma$  denotes the finite set of all state variables.
- A finite local neighbourhood set  $\mathcal{N}(c_i)$  with cardinality  $N$ .
- A transition function  $\phi : \Sigma^N \rightarrow \Sigma$  which takes local neighbour states as input. This is also known as the CA "update rule".

At each time step, the state of each cell is simultaneously updated according to the transition function. That is,  $\sigma_i(t+1) = \phi(\{\sigma_j(t) \mid c_j \in \mathcal{N}(c_i)\})$

Due to the breadth of systems studied in CA literature, the constraints of this definition are often altered to produce interesting arrangements. For example:

- The structure need not be a square grid. CA have been studied on hexagonal grids[6], aperiodic tessellations such as the Penrose tiling[7], and even randomly generated structures like the Voronoi partition[8].
- The system need not be deterministic. Probabilistic cellular automata (PCA) have stochastic transition functions which describe a probability distribution of possible outcomes for any given input. PCA are able to model random dynamical systems in the real world from stock markets[9] to infectious diseases[10].
- The state space  $\Sigma$  need not be finite. In this thesis we will explore multiple possible state variable representations including bit arrays and continuous vectors.

For the purpose of this thesis, we will assume the original definition of CA unless otherwise stated.

#### 2.1.1 Neighbourhood Functions

We consider a "neighbourhood function" for each cell  $c_i \mapsto \mathcal{N}(c_i)$ . This makes it easier to discuss neighbourhood sets of cells in the CA, each of which are typically homogenous.

There are many possible neighbourhood functions for any given CA geometry. When defining the neighbourhood function, we select a distance metric  $d : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$  to measure the proximity of two cells and we set a threshold  $T$  under which we consider two cells to be within each other's neighbourhood.

$$c_i \in \mathcal{N}(c_j) \iff d(c_i, c_j) \leq T$$

There are two neighbourhoods that are frequently used on Euclidean lattices. The *von Neumann neighbourhood* contains all cells within a Manhattan distance of 1. For a 2D square lattice, this contains the cell itself and the 4 cells in the cardinal directions. For a 3D cubic lattice, it contains the central cell and a 6-cell octahedron around it. The *Moore neighbourhood* contains all cells at a Chebyshev distance of 1. For a 2D square lattice, this is the central cell with the 8 neighbouring cells in a square around it. In the 3D case, it is a cube.

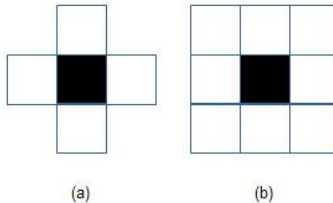


Figure 2.1: (a) von Neumann Neighbourhood and (b) Moore neighbourhood on a 2D square lattice [1]

In a finite grid CA, border cells must be given special consideration since they do not have the same number of neighbours as interior cells and therefore cannot share the same neighbourhood function. One option is to define a case-wise neighbourhood function with different behaviour for border cells. Another option is to freeze the state of border cells. In the field of partial differential equations, this is known as setting "fixed boundary conditions". The problem can also be circumvented entirely by relaxing the finite grid assumption and allowing cells to "wrap around" the grid. This is known as setting "periodic boundary conditions" and can be imagined visually as running the CA on an infinite periodic tiling or, alternatively, on a torus.

### 2.1.2 Conway's Game of Life

A popular example of a CA is the Game of Life (henceforth "Life") formulated by John Conway in 1970 [11]. It consists of a 2D grid of cells, each with a boolean state variable signifying that the cell is either "alive" or "dead". The transition rule takes as input the cell's own state  $\sigma_i(t)$  and the number of living individuals in the cell's Moore neighbourhood (excluding itself), denoted  $n$ . This is as follows:

$$\phi(\sigma_i(t), n) = \begin{cases} 0 & \sigma_i(t) = 1 \text{ and } n < 2 \text{ (Death by "exposure")} \\ 0 & \sigma_i(t) = 1 \text{ and } n > 3 \text{ (Death by "overcrowding")} \\ 1 & \sigma_i(t) = 1 \text{ and } n \in \{2, 3\} \text{ (Survival)} \\ 1 & \sigma_i(t) = 0 \text{ and } n = 3 \text{ (Resurrection)} \\ 0 & \text{otherwise} \end{cases} \quad (2.1)$$

Despite its simple setup and update rule, Life can exhibit the emergence of complex patterns. It is possible to simulate a fully universal Turing machine within Life [CITE] and, as a corollary of the Halting Problem [CITE], this means that Life is undecidable. Given two configurations, it is impossible to algorithmically determine whether one will follow the other.

Patterns found within Life include still lifes like the *block* which are fixed-point solutions to the transition function as well as periodic oscillators like the *beacon* which has period 2. There are also periodic patterns that move across the lattice such as the *glider* pattern. It is possible to discover new stable patterns by repeatedly running specific rules on random initial patterns of a pre-determined density (called soups) and classifying the objects remaining after transient reactions have dissipated. Large-scale experiments of this nature are called "soup searches"[CITE].

A CA is considered "Life-like" if it exists on a 2D lattice, has binary state, uses the Moore neighbourhood function. Life-like cellular automata exist in two varieties: inner-totalistic and outer-totalistic.

**Definition 2.2** (Inner-totalistic). *A Life-like CA is inner-totalistic if the output of the transition function depends only on the number of living cells in a cell's neighbourhood (including the cell*

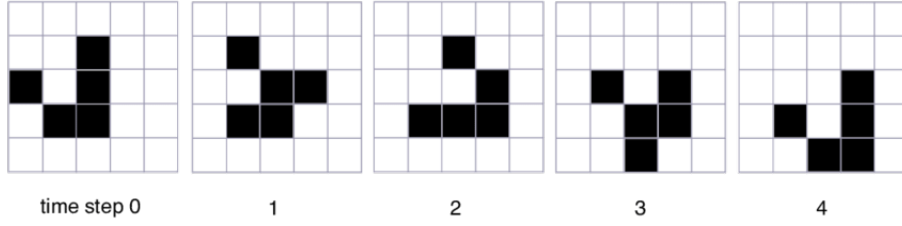


Figure 2.2: The glider pattern in the Game of Life [2]

itself).

$$\sigma_i(t+1) = \sigma_j(t+1) \iff \sum_{c_p \in \mathcal{N}(c_i)} \sigma_p(t) = \sum_{c_q \in \mathcal{N}(c_j)} \sigma_q(t)$$

**Definition 2.3** (Outer-totalistic). *A Life-like CA is outer-totalistic if the output of the transition function depends on both the number of living cells in a cell's neighbourhood and the state of the cell itself.*

$$\sigma_i(t+1) = \sigma_j(t+1) \iff \sum_{c_p \in \mathcal{N}(c_i)} \sigma_p(t) = \sum_{c_q \in \mathcal{N}(c_j)} \sigma_q(t) \quad \text{and} \quad \sigma_i(t) = \sigma_j(t)$$

As an example of the subtle difference here, consider the configurations shown in Figure 2.3. An inner-totalistic CA would yield identical configurations in the next time step since both input configurations have 3 active cells in the neighbourhood set. However, an outer-totalistic CA would treat both configurations separately as one has a live centre cell and the other has a dead centre cell. This discrepancy corresponds to a great difference in the size of search spaces. There are  $2^{10} = 1024$  inner-totalistic CA but  $2^{18} = 262144$  outer-totalistic CA. A B/S rulestring represents the transition function of an outer-totalistic CA in a form called birth-survival notation.



Figure 2.3: Two possible configurations of a Life-like CA[CITE]

**Definition 2.4** (Birth-survival notation). *Let  $N_b$  and  $N_s$  be sets of integers. We say an outer-totalistic CA has rulestring  $BN_b/SN_s$  if it has transition function:*

$$\phi(\sigma_i(t), n) = \begin{cases} 1 & \sigma_i(t) = 0 \text{ and } n \in N_b \text{ (Birth)} \\ 1 & \sigma_i(t) = 1 \text{ and } n \in N_s \text{ (Survival)} \\ 0 & \text{otherwise} \end{cases}$$

Using this notation, we can represent the Game of Life as B3/S23. In this thesis, when we refer to Life-like CA, we implicitly assume the outer-totalistic variety.

### 2.1.3 Wolfram's Classification

The choices of lattice geometry, neighbourhood function, state variable, and transition rule define the behaviour of a CA. Fixing the former three factors, Wolfram [12] classified CAs based on transition rules as follows:

1. Class 1 (Null) : Rules that lead to a trivial, uniform state
2. Class 2 (Fixed-point / Periodic) : Rules that lead to stable or periodic patterns

3. Class 3 (Chaotic) : Rules that lead to chaotic patterns
4. Class 4 (Complex) : Rules that lead to complex, long-lived impermanent patterns

**Elementary cellular automata** are defined on the simplest nontrivial lattice, a finite one-dimensional chain. The neighbourhood of each cell contains the cell itself and the two cells adjacent to it on either side. The state variable is a boolean which means there are  $2^3 = 8$  possible neighbourhood state configurations. A transition rule maps each of these neighbourhood states to a resultant state and can therefore be represented as an 8-digit binary rule table ( $t_7 t_6 t_5 t_4 t_3 t_2 t_1 t_0$ ) where configuration (000) maps to  $t_0$ , (001) maps to  $t_1$ , ..., and (111) maps to  $t_7$ . Consequently, there are  $2^8 = 256$  possible transition functions for elementary CA.

The Wolfram code, a number between 0 and 255 obtained by converting the binary rule table to decimal, is the standard naming convention for these rules. Rule 110 is particularly notable as it can exhibit class 4 behaviour [3] and is Turing complete [13]. Figure 2.4 shows an example progression of a Rule 110 system. Each row of pixels represents the state of the automaton at one snapshot in time with the topmost row representing the randomized initial state. It shows the emergence, interaction, and subsequent dissipation of multiple long-lived impermanent patterns.

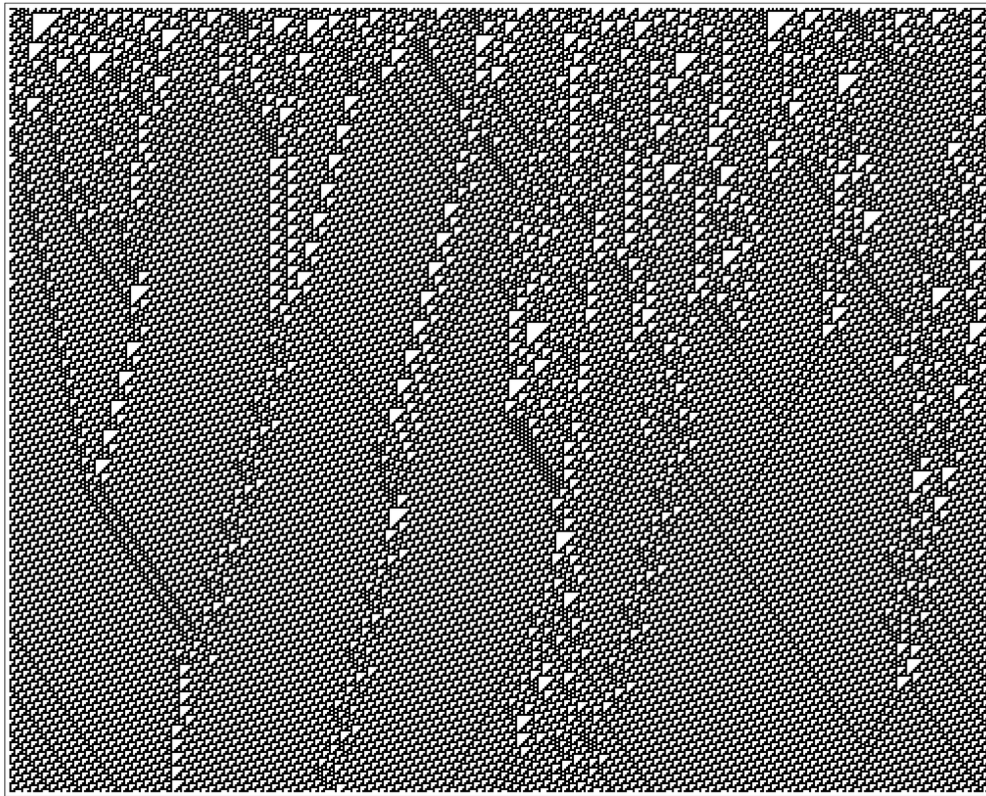


Figure 2.4: Rule 110 progression with random initialisation [3]

## 2.2 Evolutionary Algorithms

Evolutionary algorithms (EAs) are a family of heuristic-based search algorithms for black-box optimisation problems. They are inspired by biological evolution. A population of candidate solutions is initialized and modified through repeated selection, mutation, and recombination. We define an EA formally in Algorithm 1.

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### Algorithm 1 Schematic Evolutionary Algorithm

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**Require:**  $S$  - the set of possible chromosome values

**Ensure:**  $s^* \in S$

$t \leftarrow 0$

$M_0 \leftarrow \mu$  random individuals from  $S$

**while** stopping condition is false **do**

    EVALUATE( $M_t$ )

$P_t \leftarrow \text{SELECTPARENTS}(M_t)$

▷ Parents

$\Lambda_t \leftarrow \text{RECOMBINE}(P_t)$

▷ Children

$P_{mod_t} \leftarrow \text{MUTATE}(P_t)$

$\Lambda_{mod_t} \leftarrow \text{MUTATE}(\Lambda_t)$

$M_{t+1} \leftarrow \text{SELECTPOPULATION}(P_{mod_t}, \Lambda_{mod_t})$

$t \leftarrow t + 1$

**end while**

$s^* \leftarrow \text{FINDBESTCANDIDATE}(P_t)$

---

The initial selection phase ( $\text{SELECTPARENTS}()$ ) uses an objective function, also known as a fitness function, to compare and select the top candidates. Recombination produces a set of children that have similar properties to some subset of the parents. This exploits the cumulative progress of the evolutionary process embedded in the parent candidates. Mutation explores new areas of the search space by perturbing properties of the parents and children. The latter selection phase ( $\text{SELECTPOPULATION}()$ ) produces a new population from the modified parents and children. Population-wide selection criteria can be enforced in this phase. For example, certain parents can be eliminated if they have survived for too many generations or, symmetrically, children can be granted immunity for a particular number of generations.

EAs are valued for their broad applicability as they require no information about the constraints or derivative of the objective function. In fact, an explicit representation of the objective function is not even necessary to run an EA as long as candidates can be compared to each other. Selection pressure can then be introduced in the form of tournament-based elimination.

Typically, an EA acts on a population of "chromosomes" which are indirect encodings of candidate solutions. The structure of the chromosome is called the "genotype" and the structure of the corresponding solution is called the "phenotype". In this thesis, the genotype will usually be a set of parameters that characterise the transition function for a particular class of CA. The corresponding phenotype is the cellular automaton with that transition function.



# Chapter 3

## Related Works

This chapter summarises recent work on the analysis and learning of cellular automata. We focus our exploration on two classes of automata. The first are binary outer-totalistic CA, also known as life-like CA (see Def 2.3). The second are continuous reaction-diffusion CA which model simple chemical reactions. As we will see, these are a natural extension of life-like CA which, under certain constraints, themselves can be interpreted as discrete reaction-diffusion simulations with each cell accommodating the reactant or the substrate - a binary choice.

### 3.1 Binary Outer-Totalistic CA

#### 3.1.1 Exploration

Early attempts to categorise 2D cellular automata by Packard and Wolfram[14] extend Wolfram's original 4 categories. They quantify information content and rate of information transmission for particular rule subsets using metrics such as Shannon entropy and Lyapunov exponents respectively. However, these metrics do not translate to clear global decision boundaries between Wolfram's classes. As proven by Yaku[15], many questions about global properties of 2D CA are formally undecidable which makes the construction of definitions based on sets of resultant configurations difficult.

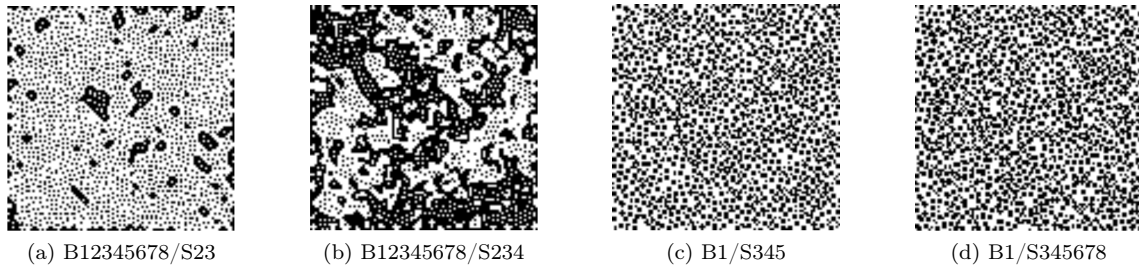


Figure 3.1: Configurations generated from P-class (a,b) and O-class (c,d) rules [4]

Adamatzky et al.[4] produces a systematic analysis of a subset of life-like CA where birth and survival sets are contiguous intervals. These are dubbed "binary-state reaction-diffusion cellular automata (RDCA)" as they provide a discretized simulation of simple substrate-reagent reactions. The analysis includes categorisations based on qualitative factors like the features and density of resulting configurations and quantitative factors like the outcome of glider collisions within each universe. For example, the **P**-class contains rules with high diffusion rate (i.e. wide birth interval) and low reaction rates (i.e. narrow survival interval) which produce large regions of 0-state and 1-state each containing scatterings of the other within them. These patterns are qualitatively distinct from, for example, **O**-class rules which have low diffusion rate and high reaction rate producing irregular spotted patterns. Despite the depth of this investigation, the 1296 CA rules analysed cover less than 0.05% of all life-like CA. A broader issue in both Wolfram's and Adamatzky's classifications is the lack of objective distinction between class boundaries which makes it difficult to predict the behaviour of rules *a priori*. Indeed, some automata have been proven to span multiple

classes[16].

This dilemma is alleviated to some degree by Eppstein’s four-way classification[5] which is based on strict definitions of *fertility* and *mortality*. A rule is fertile if there exists a finite pattern that eventually escapes any bounding box  $B$ . Note this is symmetrically opposite to the definition of periodicity since any infertile rule can only iterate through  $2^{|B|}$  steps before repeating a previous state. A rule is mortal if it supports a pattern which transitions to the *quiescent* state (i.e no live cells) in the next time step. Eppstein conjectures that "interesting" behaviour arises out of rules that are both fertile and mortal. Figure 3.2 depicts a schematic map of his analysis.

This work provides a strong theoretical foundation to guide our search of life-like CA and to verify that our techniques are effective on different varieties. However, they are not grounded in a systematic statistical search to reveal the proportion of each category that exist in contested regions. For example, we may be interested in the ratio of fertile to infertile configurations for B3/S01. Although a closed-form solution for this ratio is infeasible, it is possible to come to an approximation through simulation. Soup searches are large scale simulations of random initial conditions on particular rules typically used to identify new patterns. In a similar vein, we will use soup searches to approximate the fertility and periodicity of all rules in the life-like CA rulespace.

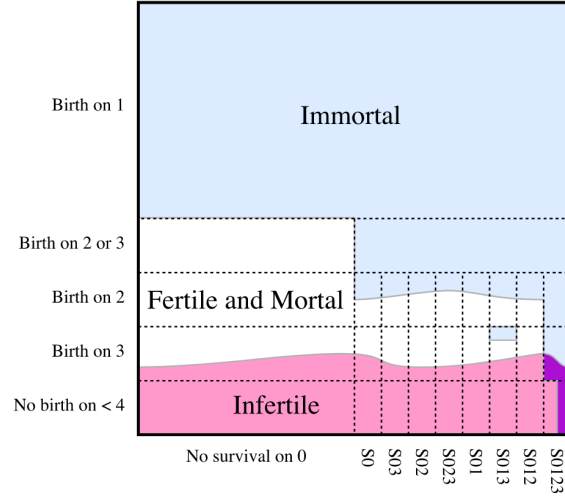


Figure 3.2: Map of fertile, infertile, mortal, and immortal regions in binary-state RDCA rulespace [5]

### 3.1.2 Learning

**Learning Algorithm for Modeling Complex Spatial Dynamics** (Meyer et al., 1989) [17] is a seminal work that uses genetic algorithms to learn cellular automata neighbourhood functions. It evolves a binary probabilistic cellular automaton (PCA) to model artificially generated datasets. The motivation is to establish a CA architecture to codify patterns in physical interactions directly from experimental data. In particular, Richards et al. [18] uses PCA rules to predict the the dendritic solidification structure of  $\text{NH}_4\text{BR}$ .

Note that the goal is not to learn the entire transition function of the cellular automaton. This work aims to establish *which* parameters in a local vicinity of a current cell are most relevant to predicting the future state, not *how* those parameters are combined and transformed to produce the result.

The search space is a 20-cell vicinity where each cell can be included or excluded from the neighbourhood set. It is the intersection of the Moore neighbourhood in time step  $t - 1$  and the von Neumann neighbourhood of range 2 in time step  $t - 2$  as visualised in Figure 3.3.

The full 20-cell neighbourhood is called the master template and each chromosome encodes



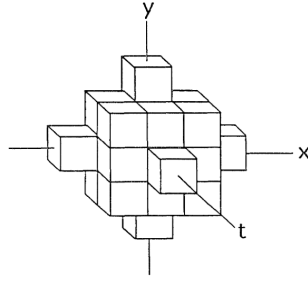


Figure 3.3: 20-cell, two step neighbourhood in space and time

some subtemplate  $s_1, \dots, s_m$ . The fitness function used is

$$F = I - \frac{2^m}{N}$$

$$\text{where } I = \sum P(s, s_1, \dots, s_m) \log_2 \frac{P(s, s_1, \dots, s_m)}{P(s)P(s_1, \dots, s_m)}$$

Here,  $I$  is the mutual information of the subtemplate and represents the amount of information, measured in Shannon bits, that can be obtained about the value of the central cell from subtemplate states. It is calculated by summing across all  $2^m$  configurations of the subtemplate in the data and across both values of  $s \in \{0, 1\}$ . The second term in the fitness function ensures that subtemplates of varying sizes are treated appropriately by proportionately penalising large subtemplates that, by nature, will contain more information.  $N = 20$  is the size of the master template

The genetic algorithm initialises the population at a randomly chosen subset of possible subtemplates. Selection is performed using a truncated linear ranking. Crossover is applied using an arbitrary cut in space-time on the master template as the crossover point. Point mutation is applied by either adding or removing a single cell from each candidate. This process is iterated to converge towards an optimum.

This method precisely learns neighbourhoods interior to the master template such as the 1 time step Moore neighbourhood. Even when the objective neighbourhood lies partially outside the master template, the algorithm successfully finds a close approximation. For example, when given data produced by a 1 time step von Neumann neighbourhood, the algorithm learns a neighbourhood set that produces correct behaviour 96% of the time.

As the first notable exploration of learning CA properties with genetic algorithms, this paper demonstrates the ability of GAs to efficiently traverse an opaque search space and approximate solutions to goals outside the search space.

This work also raises many questions for future research. The most pertinent is whether it is possible to link learned rules to existing and future theoretical models. Moreover, this work only explores binary state CA but application of similar techniques on continuous-state CA could closer approximate the partial differential equations that underlie the physical processes being modelled.

Finally, this paper focuses on optimising the neighbourhood set of the CA model only. In this thesis, we are interested in going beyond this and approximating the full transition function. In some cases we will fix the neighbourhood function used to reduce our search space under the assumption that techniques from this paper can be used to find optimal sub-neighbourhoods if they exist.

**Evolving Cellular Automata with Genetic Algorithms** (Mitchell, Crutchfield, and Das, 1996) [19] shows the effectiveness of genetic algorithms in learning elementary cellular automata for global learning tasks such as the infamous density classification[CITE] and synchronisation[CITE] problems.

## 3.2 Continuous Reaction-Diffusion CA

# Chapter 4

## Design

In this chapter we outline the workings of the evolutionary algorithm toolkit.

### 4.1 Evolutionary Algorithm Toolkit

### 4.2 Cellular Automata Simulator

# Chapter 5

## Method

### 5.1 Life-like CA

#### 5.1.1 Genetic Algorithm

#### 5.1.2 Species Analysis

### 5.2 Reaction-diffusion CA

#### 5.2.1 Evolutionary Strategies

#### 5.2.2 Particle Swarm Optimisation

## Chapter 6

# Application

### 6.1 Maze Generation

#### 6.1.1 Region Merging Algorithm

#### 6.1.2 Fitness Evaluation

#### 6.1.3 Selection and Quality-Diversity

## Chapter 7

# Evaluation

## Chapter 8

## Conclusions

## Chapter 9

# Ethical Considerations



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