The Identification of Cellular Automata

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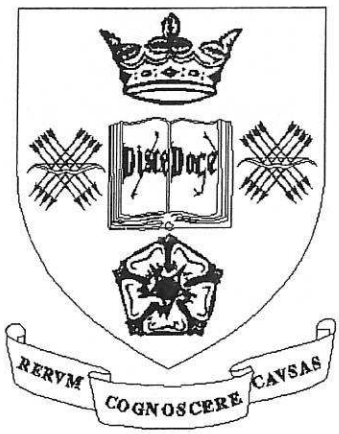

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Abstract

Although cellular automata have been widely studied as a class of the spatio temporal systems, very few investigators have studied how to identify the CA rules given observations of the patterns. A solution using a polynomial realization to describe the CA rule is reviewed in the present study based on the application of an orthogonal least squares algorithm. Three new neighbourhood detection methods are then reviewed as important preliminary analysis procedures to reduce the complexity of the estimation. The identification of excitable media is discussed using simulation examples and real data sets and a new method for the identification of hybrid CA is introduced.

1 Introduction to Identification of Cellular Automata

Cellular Automata (CA) are a class of spatially and temporally discrete mathematical systems characterized by local interactions. Because of the simple mathematical constructs and distinguishing features, CA have been widely used to model aspects of advanced computation, evolutionary computation, and for simulating a wide variety of complex systems in the real world [3], [8], [17] and [12].

In many applications the resulting CA pattern can be observed but the underlying CA rule is unknown. This would be true for example when dealing with natural systems. The key problem the observer faces is to understand how the system works, this involves

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identifying the underlying rule and then using the identified model of the system to predict the output. The theory of how CA rules can be extracted from observed patterns of spatio-temporal behavior is therefore fundamental to the study of CA. Essentially, this is an inverse problem, which means that the order of cause and effect is reversed: the observer knows the effects instead of the causes and tries to deduce the CA rule from the observed patterns. Often solving inverse problems is difficult because the problem itself can be ill posed. Because of these difficulties determining how the transition rules can be extracted from observed patterns of spatio-temporal behavior has attracted only few investigators, but if this problem can be solved, many applications may benefit from it. One of the first major contributions to this field was made by, Adamatzky, who presented a sequential and parallel algorithm to determine the local CA transition table [2], and introduced a genetic programming solution with automatically defined functions, to evolve a rule for the majority classification task for one-dimensional CA's [1]. Other authors including Richard [21], Maeda2003 [18], Veronique [26] and Sanchez [22] etc. have also made important contributions to this field.

However, the focus of the present paper is to provide an overview of the results developed at Sheffield. These include the introduction of a polynomial realization to represent CA rules, neighbourhood detection and system identification algorithms, the application of these methods in excitable media and real data sets, and the identification of hybrid CA. The paper is organized as follows. The identification of CA rules using a polynomial realization and an orthogonal least squares algorithm (CA-OLS) is discussed in Sec.2. Three new algorithms for neighbourhood detection are reviewed in Sec.3. The identification of excitable media and other real data sets are discussed in Sec.4 and a new algorithm for the identification of hybrid CA is discussed in Sec.5.

2 Identification of CA using the CA-OLS Method

Because most CA use either the *von Neumann*, the *Moore* or larger neighbourhoods in order to model systems with long-range interactions, the number of potential rules can become very large and this in turn complicates an already challenging problem. For example, a three-site one dimensional CA will have $2^{2^3} = 256$ possible rules while the number of possible rules will explode to $2^{2^9} = 1.3e + 154$ for a nine-site one dimensional

CA. It is therefore often very difficult to scan all the possible rules even using modern computers. To simplify the problem, Yang and Billings [27]-[28] showed that CA binary rules can be realized using a simple polynomial model with the advantage that this simplifies the identification problem. Based on this idea, they proposed the CA-OLS method which can determine the CA neighbourhood and the unknown model parameters.

2.1 Boolean Form of CA Rules

The local rule for a binary cellular automata may also be considered as a Boolean function of the cells within the neighbourhood. For a 1-D CA, denote the state of the cell at position j at time step t as $s(j;t)$ and the states of the cells within the neighbourhood of cell j at previous time steps as $N(j;|t)$ where $|t$ represents time steps before t. The 1-D CA can then be represented by

$$s(j;t) = f(N(j;|t)) \tag{1}$$

where f is the Boolean form of the local transition rule.
According to [28], every CA with an n site neighbourhood $cell(x_1;|t), cell(x_n;|t)$ may be written as

$$s(x_j;t) = a_0 \oplus a_1 s(x_1;|t) \oplus \cdots \oplus a_N(s(x_1;|t) * \cdots * s(x_n;|t)) \tag{2}$$

where $N = 2^n - 1$ and cell $(x_j;t)$ is the cell to be updated.
Equation (2) is important because it significantly reduces the complexity of CA identification by using a reduced set of logical operators. The difficulty in identifying multi-dimensional CAs is also decreased because the higher dimensional CA rules are reduced to an equation which depends on the size of the neighbourhood not the dimensionality.

2.2 Polynomial Form of CA Rules

Every CA with an n site neighbourhood can be reformulated from a truth table to a Boolean function of the form of Eq. (2). However, the model to be identified is defined in terms of AND and XOR operators and is therefore nonlinear in the parameters. However, it is often advantageous to reconfigure the nonlinear model to be linear in the parameters if this is possible.

If a,a_1,a_2 are binary integer variables taking the values 0 and 1 for true and false, respectively, then there is an exact polynomial representation of each of the logical functions

$$\begin{aligned} a_1 \oplus a_2 &= a_1 + a_2 - 2a_1 \times a_2 \\ a_1 \times a_1 &= a_1 \end{aligned} \tag{3}$$

Therefore, all CA rules can be represented by an exact polynomial expressions. Moreover, using the Principle of Duality and Absorption in Boolean Algebra where for every binary variable a, $a \times a = a$, considerable simplification can be achieved. Hence, a general polynomial expression of all binary CA rules with an n-site neighbourhood $\{cell(x_1;|t), ..., cell(x_n;|t)\}$ can be expressed by the exact polynomial expression

$$s(x_j;t) = \theta_1 s(x_1;|t) + \cdots + \theta_n s(x_n;|t) + \cdots + \theta_N s(x_1;|t) \times \cdots \times s(x_n;|t) \tag{4}$$

where $N = 2^n - 1$ and cell$(x_j;t)$ is the cell to be updated. Using this important observation the number of parameters to be identified can be substantially reduced to only $2^n - 1$. It can also be seen that the most important factor is the size of the neighbourhood n, not the order of the dimension.

2.3 Identification using the CA-OLS method

Based on the form of the polynomial model, an algorithm called the CA-OLS was introduced to detect the significant terms and estimate the related coefficients. The CA-OLS algorithm was derived by applying a modified Gram-Schmidt orthogonalisation procedure to Eq.(4). Full details of the CA-OLS algorithm are given in [28]. For a 3-D CA, for example, the number of possible candidate terms can be excessive, but simulations by many authors show that often complex CA patterns can be produced using simple models. If the appropriate model terms that are significant can be selected therefore all other model terms can be discarded without a deterioration in model precision or prediction accuracy and a concise CA model can be obtained. One way to determine which terms are significant or which should be included in the model can be derived as a by-product of the CA-OLS estimation algorithm and is very simple to implement. From [28], the quantity referred to as the Error Reduction Ratio (ERR) can be used to measure the contribution that each candidate term makes to the updated state $s(i,j,l;t)$ and this provides an indication of which terms to include in the model. Using the ERR

the candidate model terms can be ranked in order of importance and insignificant terms can be discarded by defining a cutoff value ct, below which terms are considered to contribute a negligible reduction in the mean-squared error. The threshold value of ct for the CA model can be set as zero because the polynomial model is not an approximation but an exact representation of the CA rules.

2.4 Identification of Probabilistic CA

Probabilistic cellular automata (PCA), which are referred to as stochastic cellular automata by some authors, are constructed by introducing probabilistic elements into deterministic local CA rules. The identification of PCA consists of determining the probabilistic local transition rules and the associated neighbourhood over which the rule is operated, from a given set of spatio temporal patterns generated by the PCA evolution. In [27], the identification of PCA was studied using a two stage neighbourhood detection algorithm. It is shown that a binary probabilistic cellular automaton (BPCA) can be described by an integer-parameterized polynomial corrupted by noise. Searching for the correct neighborhood of a BPCA is then equivalent to selecting the correct terms, which constitute the polynomial model of the BPCA, from a large initial term set. It was proved by Yang ans Billings [27] that the contribution values for the correct terms can be calculated independently of the contribution values for the noise terms. This allows the neighborhood detection technique developed for deterministic rules in [28] to be applied with a larger cutoff value to discard the majority of spurious terms and to produce an initial pre-search for the BPCA neighborhood. A multi-objective genetic algorithm (GA) search with integer constraints can then be employed to refine the reduced neighborhood and to identify the polynomial rule which is equivalent to the probabilistic rule with the largest probability. A probability table representing the BPCA can then be determined based on the identified neighborhood and the deterministic rule.

2.5 Fast CA-OLS

As shown in above sections, OLS is a core algorithm for the identification of CA. To improve the efficiency, Mei [19] proposed a fast CA-OLS (FCA-OLS) algorithm combining the ideas in [30] and [35]. The orthogonalisation was carried out using simplified

iterations instead of time expensive computations at every step. The modified algorithm is computationally less expensive.

The detail of this algorithm is given in [19]. Table 1 shows that the new FCA-OLS routine results in a significant reduction in the computational time.

Table 1: Comparison of computational cost

Data points	Dimension	neighbourhood	Time(CA-OLS)	Time (FCA-OLS)
500	1	3	100%	47.61%
1000	2	5	100%	46.87%
5000	3	7	100%	46.01%

2.6 Conclusions

The estimation procedures discussed above exploit the observation that binary CA rules can be exactly represented as polynomial models which collapse to relatively simple forms even for high-dimensional CAs. This transforms the problem from a nonlinear-in-the-parameters to a linear-in-the -parameters formulation. The only information required to initialise the algorithm is to set the range of the largest expected neighborhood over which the algorithm searches for candidate model terms. The CA-OLS estimator then searches through all the possible terms and discards all the redundant terms to yield the final estimated model.

Several simulated examples in [27], [28] show the power of the new approaches and demonstrate for the first time how polynomial CA models can be extracted from data generated from deterministic, probabilistic and high-dimensional CA systems. The simulation examples in [19] show the proposed fast CA-OLS can improve the effectiveness substantially, and this may assist further research into real-time identification for real systems.

3 Neighbourhood Detection

3.1 Background and Motivation

In most former studies, the CA neighbourhood was manually predefined as the cells that were immediately close to the cell to be updated. For example Richards directly selected the Moore structure as the neighbourhood of the pattern generated by dendritic solidification [21]. Adamazky set a minimal neighbourhood before the identification of a one-dimensional CA [2]. But for most systems, especially higher order CA, it will often be very difficult to manually choose a candidate neighbourhood that just covers the exact neighbourhood and which rejects many possible redundant cells. Hence, the detection of the significant neighbourhood before identifying the rule is a key step in CA identification.

3.2 Neighbourhood Detection using CA-OLS

As shown in Sec.2, Yang and Billings proposed the CA-OLS to detect the neighbourhood based on the polynomial realization (4) [27]-[28]. The preliminary step in this algorithm involves choosing an initial candidate neighbourhood, which can be coarse but must be large enough to include all correct neighbourhoods. Consider a one-dimensional CA for example and assume the neighbourhood of the cell $c(j;t)$ is chosen as $\{c(j-1;t-1), c(j;t-1), c(j+1;t-1)\}$, a polynomial model, expressed as equation (5), can be generated according to equation (4).

$$\begin{aligned} c(j;t) &= \theta_0 + \theta_1 c(j-1;t-1) + \theta_2 c(j;t-1) \\ &\quad + \theta_3 c(j+1;t-1) + \theta_4 c(j-1;t-1)c(j;t-1) \\ &\quad + \theta_5 c(j-1;t-1)c(j+1;t-1) \\ &\quad + \theta_6 c(j;t-1)c(j+1;t-1) \\ &\quad + \theta_7 c(j-1;t-1)c(j;t-1)c(j+1;t-1) \end{aligned} \tag{5}$$

Determining which terms are significant and which terms are redundant can be derived directly from the Error Reduction Radio (ERR), which measures the contribution of each candidate term to the updated cell, and which is part of the CA-OLS routine. Using ERR the candidate terms can be ranked in order of importance and the insignificant

terms can then be discarded.

3.3 Neighbourhood Detection based on a Statistic

Mei and Billings [20] recently proposed a new neighbourhood detection routine, which can refine the candidate neighbourhood according to a statistic associated with each combination of candidate neighbourhood cells and the updated cell, and from which an exact neighbourhood can be obtained.

The basis of this algorithm is to select a neighbourhood candidate set initially, which must be large enough to include all potential neighbourhood cells. Then each cell in the neighbourhood candidate set will be assessed according to the contribution made to the cell to be updated. Consider a one-dimensional deterministic CA for example and assume the neighbourhood of the cell $c(j;t)$ is chosen as $R_k\{c(j;t)\}$ at iteration time step k. The cells of the considered neighbourhood could be divided into two parts: confirmed cells and unconfirmed cells. A series of data pairs can be collected as $(R_k\{c(j;t)\}, c(j;t))$. Consider one of the unconfirmed cells in $R_k\{c(j;t)\}$. If it is a redundant cell based on the statistic of collected data pairs (see [20] for full details), this cell should be discarded and the data pairs should be re-collected because of the change of candidate neighbourhood. If it is a significant cell, the cell would be moved into the set of confirmed cells, and the next unconfirmed cell would be considered. This procedure is repeated until all cells in the candidate neighbourhood are confirmed.

3.4 Neighbourhood Detection using Mutual Information

All previous methods need an initial candidate set before neighbourhood detection can commence and this must include all the correct neighbourhoods. This maybe difficult for some unknown systems. To avoid this step, a new neighbourhood detection algorithm was introduced by Zhao and Billings [31] based on mutual information (MI) to provide an initial indication of the temporal and spatial range in the identification of CA. This initial neighbourhood is then used to prime a FCA-OLS algorithm to find the correct model terms and unknown parameters in a CA model. This provides a coarse-to-fine identification approach for CA where the mutual information is used to significantly re-

duce the potential neighbourhood choices which are then optimised using the FCA-OLS identification algorithm.

Consider the one-dimensional CA case to illustrate the approach and assume the neighbourhood of the cell $c(j;t)$ is $\{c(j-a_1;t-b_1),...,c(j-a_n;t-b_n)\}$. The aim is to determine the maximal spatial lag a_n and the maximal temporal lag b_n.

Definition 1 *A* ***case*** *is defined as a pair of* $\{f(R\{j;t\}),c(j;t)\}$, *where* $R\{j;t\}$ *is the neighbourhood of a cell* $c(j)$ *at time step* t *and the* $c(j;t)$ *is the state value of the cell at time step* t, *and* $f(R\{j;t\}) = c_1+2c_2+..+2^{m-1}c_m$ *assuming* $R\{j;t\} = \{c_1,c_2,...,c_m\}$. *For example, if the state value of the updated cell* $c(j;t)$ *is* 1 *and the state of its neighbourhood* $R\{j;t\}$ *is* $\{0,1,1\}$, *the* ***case*** *can be described as* $\{5,1\}$.

Essentially, $R\{j;t\}$ represents the input and the $c(j;t)$ represents the output of a non-linear system. If the candidate neighbourhood $R\{j;t\}$ is large enough to cover all the correct neighbourhoods, the mutual information between $f(R\{j;t\})$ with $c(j;t)$ should be close to 1. If $R\{j;t\}$ can not contain all the correct neighbourhoods, the Mutual Information between $f(R\{j;t\})$ with $c(j;t)$ will be close to 0. Based on these results a new criteria, which introduces MI as a fitness function to establish a measurement for ranking each candidate neighbourhood was introduced in Zhao and Billings [31].

3.5 Conclusions

Three new neighbourhood detection methods have been derived for both deterministic and probabilistic CA. Yang's method directly selects the significant terms by the ERR values, the by-product of CA-OLS, but the procedure can be time consuming if the candidate neighbourhood is large. Mei's method allows the neighoubhood detection to be decoupled from the CA rule determination by choosing the exact neighbourhood. Essentially, this is a preliminary step before Yang's method, which may save time when implementing CA-OLS. Zhao's method solves the problem of initial neighbourhood selection and produces an exact neighbourhood as well.

Many simulation examples have been given in the corresponding papers to demonstrate the effectiveness of all three methods and the results are encouraging.

4 Identification of Excitable Media

4.1 Introduction

Excitable media systems, which were first introduced by Wiener and Rosenbluth in order to explain heart arrhythmia caused by spiral waves [23], are now recognized as an important class of spatio-temporal dynamic systems. Examples of excitable media systems include the Belousov-Zhabotinskii (BZ) reaction [16], waves of electrical stimulation in heart muscles [25], autocatalytic reactions on metal surfaces [15], and the propagation of forest fires [9].

Wiener introduced the notation of *refractory state*, *excited state* and *excitable state* to investigate excitable media. The defining characteristics of excitable systems are: starting at a stable equilibrium (excitable state) a stimulus above a certain threshold generates a burst of activity (excited state) followed by a refractory period. Due to the activity initiated by a supercritical perturbation, travelling excitation waves of various geometries can occur, including ring and spiral waves.

In this section the focus is on developing algorithms which can be applied to determine the neighbourhood and a representative model of excitable media from observations of the spatio-temporal pattern and no other *a priori* information. The study begins with examples of excitable media behaviour to demonstrate that highly complex patterns, can be generated from relatively simple models. A algorithm using mutual information is then derived to determine the neighbourhood, the excitation threshold, and the number of excitation states. Based on the above steps two methods of identifying the rule based on a multimodel and a polynomial model representation are introduced.

4.2 Simulation of Excitable Media in CA

The Greenberg-Hasting Model(GHM), which was introduced by Greenberg and Hasting [14], is the most common CA form of model for excitable media.

The GHM model γ_t is a very simple cellular automata that emulates an excitable media [Robert, 1993]. At each time t, $\gamma_t \in \{0, ..., N-1\}^{\mathbb{Z}^d}$. This means that for each $x \in \mathbb{Z}^d$, $\gamma_t(x)$ has one of N possible values $0, ..., N-1$. The evolution of the GHM model can be determined by three parts: a discrete lattice, a finite neighbourhood $\mathcal{R}$, and a transition

rule.

For the GHM, the commonly used type of lattice is the square lattice. The neighbourhood structure varies depending on the construction of the model. Consider a two-dimensional GHM as a CA for example. The neighbourhood could be a *von Neumann* structure, a *Moore* structure or an *Extended Moore* structure [32].

The transition rule of a GHM can be determined by three parameters: the number N of all available states; the number E of excited states; the threshold number T of sites needed for excitation. Denoting the cell at position (x, y) at time step t as $c(x; y; t)$. The state $c(x; y; t)(c(x; y; t) \in \{0, ..., N-1\})$ is an integer value, where 0 represents an excitable state, $1, ..., E$ represent the excited states, and $E+1, ..., N-1$ represent the refractory states. Initializing each cell at time step 0, the GHM updates all cells synchronously by **Transition Rule 1** at each step.

Transition Rule 1 *The transition rule of the GHM as a CA:*

- *if* $1 \leq c(x; y; t) < N$, *then* $c(x; y; t+1) = (c(x; y; t) + 1) \ mod \ N$
- *if* $c(x; y; t) = 0$, *then* $c(x; y; t+1) = 1$ *when* $\#(\mathcal{R}_{c(x;y;t)}) \geq T$, *else* $c(x; y; t+1) = 0$ *($\mathcal{R}_{c(x;y;t)}$ denotes the neighbourhood of $c(x; y; t)$, $\#(\mathcal{R})$ denotes the number of excited sites in $\mathcal{R}$)*

Using this simple rule, different complex patterns can be generated using different initial values or parameters. Figure 1 shows an example generated by GHM.

4.3 Identification of Excitable Media

There are two parameters that need to be determined during the identification of excitable media: the neighbourhood and the transition rule. In the following sections algorithms to detect the neighbourhood and to identify the rule will be discussed.

4.3.1 Neighbourhood detection

For most systems, especially high dimensional CA, it will be very difficult to manually select an appropriate candidate neighbourhood that just covers the exact neighbourhood and rejects the redundant cells. This will be particularly true for two-dimensional CA,

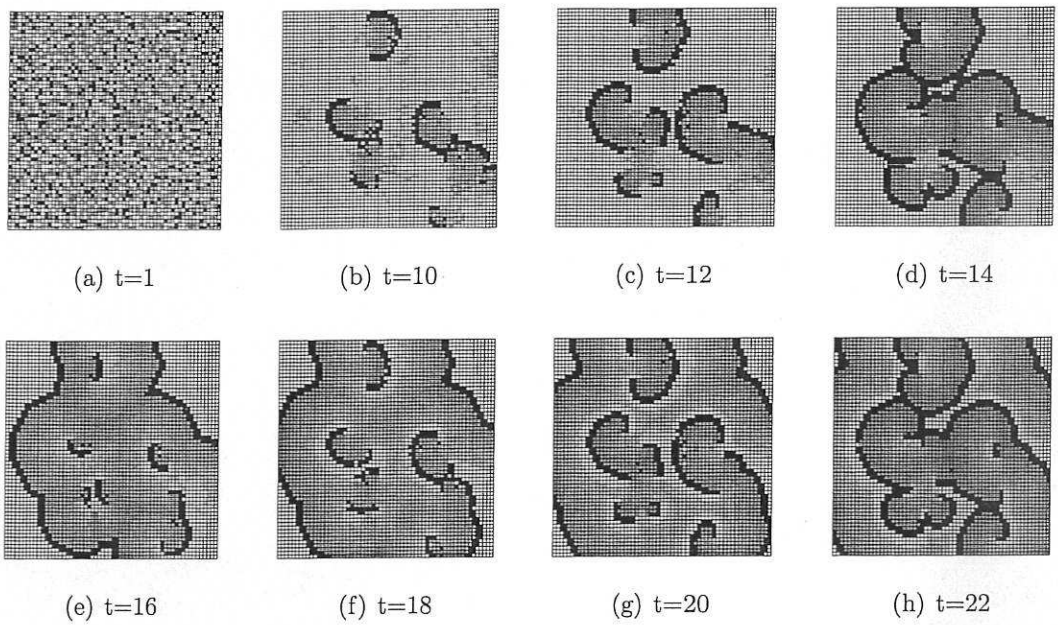


Figure 1: Evolution of a GHM as a CA on a 60×60 square lattice with an Extended Moore neighbourhood($r = 2$), and $N = 7$, $E = 1$ and $T = 3$.

such as excitable media systems. If an incorrect neighbourhood is selected, it will either be impossible to find the correct model or the model will be over parameterized and computational time will increase dramatically. Based on the special properties of excitable media, a new neighbourhood detection approach has been introduced based on mutual information, which can not only determine the neighbourhood but also estimate the number E of excited states [32].

The neighbourhood detection procedure can be briefly summarized by the following steps.

Initially select the candidate neighbourhood as the *von Neumann* neighbourhood and select E as 0.

1. Threshold all the observed patterns to create a binary pattern using the current E.

2. Scan all the binary patterns and calculate the value of the mutual information.

3. Increase E and repeat *steps 1* and *2* until $E = n$, where n denotes the number of current candidate neighbourhood cells.

4. Increase the candidate neighbourhood range, for example, from the *von Neumann*

structure to the *Moore structure* or from the *Moore structure* to the *Extended Moore structure* ($r = 2$) and reset E to 0. Then repeat *steps 1* to *3* until a peak value of mutual information appears. The candidate neighbourhood and E with maximal mutual information can be determined as the final results.

4.3.2 Rule identification

Two types of models, the multiple model and the polynomial model, can represent the transition rule of excitable media, and algorithms for the identification both of these have been proposed.

Rule identification using a multiple model: The advantage of this type of model is the principle of the evolution can easily be understood and it is not difficult to simulate the model. The evolution of a GHM is determined by four parameters: the neighbourhood; the number N of all available colours; the number E of excited colours; and the threshold number T of sites needed for excitation. The selection of the neighbourhood and E have been described using mutual information above, and only N and T are unknown parameters. The estimation of N can often be ignored here because the evolution of a GHM mainly depends on the excitation from excitable cell to excited cell, and it is not important how many refractory states exist. The threshold number T therefore is the only parameter needed to be estimated in this step. The detail about how to identify T can be found in [32].

Rule identification using a polynomial model: The main advantage of the polynomial model form is that it is much easier to analyse and validate than the multiple model. After generating binary frames using the detected value of E, the identification of the rule using a polynomial representation can be summarized as:

1. Collect the input-output cases $\{x_i; y_i\}, i \in \{1, ..., M\}$ using the detected neighbourhood and E, where

$$\begin{aligned} x_i &= \{c(x - a_1; y - b_1; t - 1), c(x - a_2; y - b_2; t - 1), ..., c(x - a_n; y - b_n; t - 1)\} \\ y_i &= c(x; y; t) \end{aligned} \tag{6}$$

   M denotes the number of collected cases and n denotes the number of neighbourhood cells.

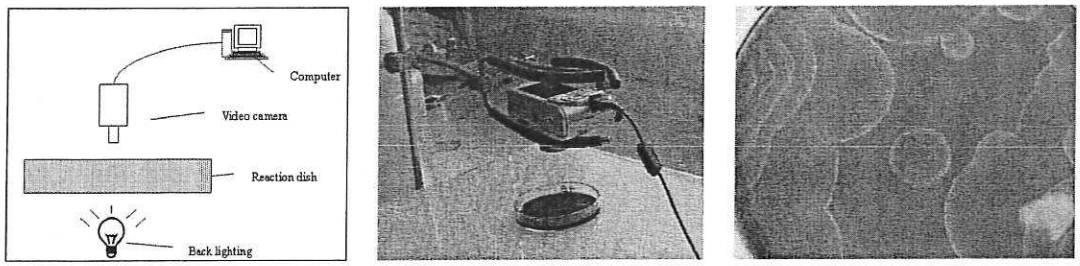
2. Apply the Orthogonal Least Squares (OLS) algorithm for CA to estimate the parameters of Eq. (4) using the collected data set $\{x_i; y_i\}$.

4.4 Identification of a Belousov-Zhabotinsky Reaction using CA Models

4.4.1 Introduction

The Belousov-Zhabotinsky (BZ) chemical reaction, named after B.P.Belousov who first discovered the reaction [10] and A.M.Zhabotinsky who continued Belousov's early work [29], is a famous experiment in excitable media. Once the reaction gets started grey rings and spirals can be seen propagating from localized regions on a red background. A snapshot of a typical pattern is shown in Fig.2.(c), where the wave fronts of the observed patterns appear to be quite similar to those of the simulated patterns using the GHM, especially the pattern shown in Fig.1.

In this section the identification of a model of a real BZ reaction using a CA model



(a) (b) (c)

Figure 2: (a) Schematic of the data acquisition setup; (b) Photo of acquiring device ; (c)A snapshot of an acquired pattern

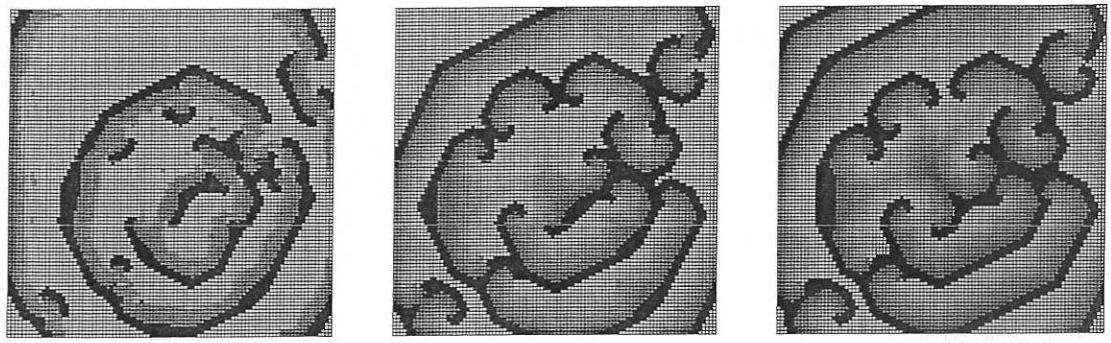
directly from sampled data will be studied. The focus of the section will be on the practical aspects of imaging a real BZ reaction and the identification of dynamic models of this system because there are very few results on these type of problems in the literature.

4.4.2 Data acquisition and pre-processing

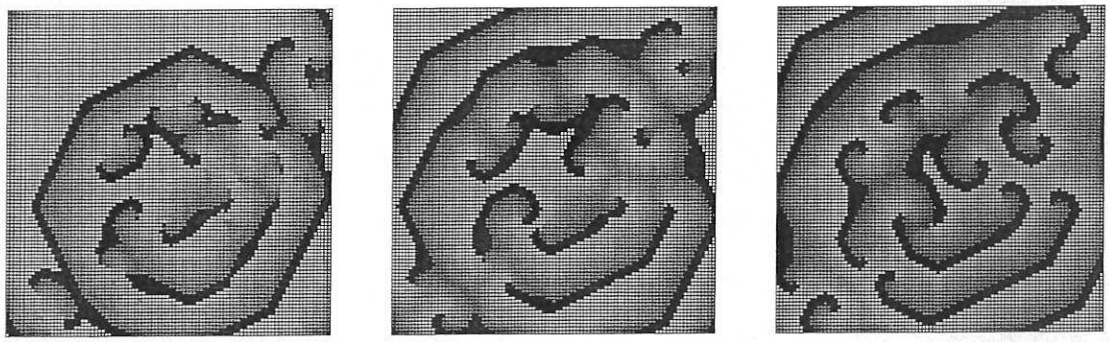
The chemical processor was prepared in a thin layer BZ reaction using a recipe adapted from Field and Winfree [24]. The experimental apparatus of acquisition is illustrated by Fig.2.(a). To acquire the high quality images a digital camera, which was fixed by a bracket and connected to the computer directly using the USB socket as shown in Fig.2.(b), was used. The images were acquired with 640×480 pixel resolution where each pixel had a 24bit colour-scale value. Before identification the acquired raw data must be pre-processed to reduce noise and must then be mapped onto a lattice based on the three components of CA, which involves the calibration of the pixel size and the calibration of the number of colours. The detail of these steps can be found in [33].

4.4.3 Rule identification

Region selection: In most recent studies of excitable media the evolution of the pattern is assumed to be uniform so that each cell in the pattern has the same transition rule. This may not hold for a real system because there may be noise introduced by data acquisition which could make the rule change. Hence, it is necessary to select an appropriate region of the image which has a uniform or nearly uniform rule. A method was proposed in [33] which divides the image into n_s squares, and then estimates the threshold number T in the GHM of each part. Normally, n_s was chosen as 64 for a raw image with 640×480 pixels. Part of the image can then be chosen as the sample area where the rule is assumed to be uniform based on the generated rule distribution graph.
Rule identification: The identification of the rule for the considered region of the BZ reaction is the same as the method for excitable media.
Model evaluation: To evaluate the identified models visually and quantitatively, One Step Ahead (OSA) predictions were compared with the recorded data. Figure 3.(a)-(c) visually shows the $10, 50, 80$ time step OSA predictions using the identified multiple model, and Fig.3.(d)-(f) show the $20, 60, 100$ time step OSA predictions using the identified polynomial model. Both these clearly demonstrate the diffusion characteristics of the BZ patterns. To quantitatively access the performance of the obtained CA rules we can compare the results of the predictions from the identified models to the actual BZ evolution at a certain time step. To achieve this a correlation coefficient, which takes



(a) 10 steps (b) 50 steps (c) 80 steps



(d) 20 steps (e) 60 steps (f) 100 steps

Figure 3: (a)-(c):OSA predictions using the identified GHM; (d)-(e):OSA predictions the identified polynomial model

into account the correct and false cell predictions for the excited state and refractory state, and the correct and false cell predictions for the excitable state are used. Full details of these procedure can be found in [33].

4.5 Conclusions

New methods of extracting mathematical models of CA directly from real imaged data from a BZ reaction has been presented. A procedure which maps the digital image to a latticed CA pattern has been proposed. New methods of synthesizing the horizontal and vertical calibration were introduced, together with the edge purging procedure to remove the gradient between the wave fronts and the background. A new region selection approach has also been proposed, and procedures for the identification of two CA model types, the GHM and the polynomial model, have been described. A comparison of the predictions with the actual patterns both visually and quantitatively shows that the

results are very encouraging. The identified models can reproduce the patterns with similar dynamic features compared to the actual BZ reaction.

Identification of real reaction systems is often very difficult because of the many factors involved. Moreover, natural data will always be slightly corrupted by the imaging devices during data acquisition. The results in the section represent preliminary results and many more experiments need to be conduced and all aspects of the data collection and modelling of this complex class of system require further study.

5 Identification of Hybrid Cellular Automata using Segmentation Methods

Most previous investigations of CA have concentrated on uniform cellular automata, or CA where the transition rule is identical at all positions over the whole lattice and at all times during the evolution. However, when studying an unknown real system, it may be unwise to assume that the rule representing the system is homogeneous over the whole image. Hence, recently, the application of hybrid cellular automata has attracted more and more investigations [11]-[13], which try to represent a complex system using multi-rules. However, very few of these methods can solve the inverse problem - that is identifying the hybrid cellular automata rule given the observed data.

This section introduces a new method for the identification of hybrid CA which initially simplifies the problem from hybrid CA to uniform CA by partitioning the regions based on the rules by employing the segmentation methods. Then the methods described in previous sections can be applied for the identification of CA with a uniform rule in each separate region to obtain the final hybrid rule or model.

The procedure of transferring the identification of hybrid CA to the identification of uniform CA can be summarized by the steps in the following sections.

5.1 Map the realistic CA pattern to a virtual image.

An image is composed of pixels on a lattice, and a CA is composed of cells on a lattice, which makes the possibility of applying segmentation methods from image processing to the identification of hybrid CA.

The key step is that a pixel in a virtual image can be created by mapping a rectangular region with size $n_b \times n_b$ in the CA pattern, and this will be refereed to as a *block*. Consider a CA pattern on a $n_x \times n_y$ lattice, a virtual image with $\frac{n_x}{n_b} \times \frac{n_y}{n_b}$ pixels could be generated by setting the size of block as n_b. The selection of n_b is important because if n_b is selected to be too large, then obviously the segmentation would be less accurate and the probability of multi-rules in one block may be large. This in turn could lead to the difficulty in calculating the property of the block. If n_b is selected too small, the sample data for calculating the property of the block will be less, which could make the result over-estimated.

The method proposed in this section introduces a parameter named T_u, which represents a noise-immune ability. Consider a block which has n rules denoted by $r_1, r_2, ..., r_n$. If there is a rule r_i whose percent of occupancy in that block is larger than T_u, this block will be marked as obeying r_i. If there is no such rule, this block should be marked as unidentifiable. Obviously, T_u should be chosen between 0.5 to 1. The smaller T_u is, the more probability there is of identifying the block, but there is more risk of getting a wrong rule. Hence, there is a clear tradeoff between the accuracy of segmentation and the property calculations, and a tradeoff in the block property between the accuracy and the identifiability. The crucial step of the mapping procedure is how to calculate the property of each block in a CA pattern. The detail of this method could be found in [34]. Finally, the mapping procedure between the pattern of hybrid CA and the virtual image can be summarized as:

Consider a $n_x \times n_y$ hybrid CA pattern and denote the selected block size as n_b. If the currently considered block is identifiable, the property of the considered pixel in the image is assigned the value P_v of the corresponding block. If the block is unidentifiable, the property of the corresponding pixel in the image should be assigned a special value, such as 0. The size of the mapped virtual image would be $\frac{n_x}{n_b} \times \frac{n_y}{n_b}$.

5.2 Region Segmentation

Two popular image segmentation methods are introduced in the following sections to assist the identification of hybrid CA by partitioning the generated virtual image into some regions based on different rules.

The objective of segmentation is to partition an image into regions. This section discusses the segmentation techniques that are based on finding the regions directly. Let R represent the entire image region. The segmentation may be viewed as a process that partitions R into n subregions, $R_1, R_2, ..., R_n$, such that

$$\begin{aligned}
&(a) \quad \bigcup_{i=1}^{n} R_i = R, \\
&(b) \quad R_i \text{ is a connected region}, i = 1, 2, ..., n, \\
&(c) \quad R_i \cap R_j = \phi \text{ for all } i \text{ and } j, i \neq j \\
&(d) \quad P(R_i) = \text{ TRUE for } i = 1, 2, ..., n, \\
&(e) \quad P(R_i \cup R_j) = \text{ FALSE for } i \leq j,
\end{aligned} \tag{7}$$

where $P(R_i)$ is a logical predicate defined over the points in set R_i, and ϕ is the null set. Condition (a) indicates that the segmentation must be complete; that is, every pixel must be in a region. The second condition requires that points in a region must be connected. Condition (c) indicates that the regions must be disjoint. Condition (d) deals with the properties that must be satisfied by the pixels in a segmentation region. In the current application, $P(R_i) = TRUE$ implies the pixels in the region R_i have the same properties. Finally, condition (e) indicates that regions R_i and R_j are different in the sense of predicate P.

5.2.1 Region Growing

Region growing is a well known technique for image segmentation. It postulates that neighbouring pixels within the same region have similar intensity values. The general idea of *region growing* is to group pixels with the same or similar intensities to one region according to a given homogeneity criterion. More precisely, *region growing* starts with a set of pre-specified seed pixel(s) and grows from these seeds by merging neighbouring pixels whose properties are most similar to the pre-merged region. Typically, the homogeneity criterion is defined as the difference between the intensity of the candidate pixel and the average intensity of the pre-merged region. If the homogeneity criterion is satisfied, the candidate pixel will be merged to the pre-merged region. The procedure is iterative: at each step, a pixel is merged according to the homogeneity criterion. This process is repeated until no more pixels are assigned to this region. The homogeneity criterion in this application is the transition rule.

5.2.2 Region Splitting and Merging Method

The procedure discussed in the previous section grows regions starting from a given set of seed pixels. An alternative is initially to subdivide an image into a set of arbitrary, disjoined regions and then merge and/or spit the regions in an attempt to satisfy the conditions stated in Equation (7). A *region splitting and merging* algorithm that iteratively works toward satisfying these constraints is explained as follows.

Let R represent the entire image region and select a predicate P as discussed in Equation (7). For a hybrid CA, $P(R_i)$ =TRUE means all the cells in R_i have the same CA transition rule. Assume a square image, one approach for segmentation of R is to subdivide it successively into smaller and smaller quadrant regions such that, for any region R_i, $P(R_i)$ =TRUE. That is, if $P(R_i)$ =FALSE, the image is divided into quadrants. If P is FALSE for any quadrant, that quadrant is subdivided into sub-quadrants, and so on.

5.2.3 Removing noise

A popular nonlinear filter in image processing called the *median filter* can be employed to remove noise in the segmented image. The *Median filter* replaces the considered pixel value by the median of the values in a neighbourhood of that pixel. This method is particularly effective when the noise pattern consists of strong, spike-like components. When n_b is chosen small, there could be some blocks which can not be identified because the number of measurements is small compared to the number of possible discrete states. For this reason, the segmented image could include salt-pepper noise. *Median filtering* can remove this kind of noise effectively.

5.3 Conclusions

Some examples, including one-dimensional CA and two-dimensional CA, have been employed to evaluate this method [34]. It is shown that the results are encouraging by comparing the original rule distribution graph and the detected rule distribution graph, and comparing the comparison the reconstructed patterns and the observed patterns.

Moreover, the hybrid cellular automata could be more complex than what is described in this paper. For example, the rule could be changed in the same position following the evolution. What the paper presents are preliminary results and further investigations

are required to deal with the more complex cases which could occur in the real systems.

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