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Analysis of a method for constructing a cellular automaton from a continuous system

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Abstract

A method of constructing a cellular automaton (CA) from numerical solutions of a given partial differential equation (PDE) is considered. It consists of two parts, namely, collecting spatiotemporal data numerically and finding local rules of a CA that appear most frequently. In this paper, we analyze the method mathematically to examine its selectivity and its robustness of the derived local rules so that we can ensure validity of the resultant CA model. In particular, we investigated two limit cases: (a) the number of states of CA goes to infinity and (b) the number of spatiotemporal data goes to infinity. In the former case, we prove that the resultant CA converges to the difference equation where numerical solutions of a PDE are collected. In the latter case, through mathematical analysis, we derive conditions that the resultant CA is uniquely determined when the method of constructing a CA is applied to the diffusion equation. Our study can be a theoretical foundation of empirical CA modeling methods to create a reasonable CA which can somehow reproduce the original behavior of datasets under consideration.

Keywords: Cellular automata, Partial differential equations, Empirical methods of CA construction

1 Introduction

A method of constructing a cellular automaton (CA) from observation data of laboratory experiments was proposed by Kawaharada and Iima [2]. The essential part of the method is to find local rules of a CA that appear most frequently in spatiotemporal data of an experiment. They attempted to find a CA model for some phenomenon whose governing equation is unclear. They applied it to a pattern formation of *Euglena gracilis* and reproduced some features of the original pattern [6]. Throughout this paper, we call their method *the experimental method*, as it is based on observation data collected by an experiment to generate the local rules. The experimental method is significantly advantageous because it is applicable to any dynamical system once a sufficiently large spatiotemporal dataset is given: one can always obtain some CA.

Kawaharada and Iima [3] numerically solved an initial-boundary value problem of a partial differential equation (PDE) with random initial conditions many times by using the explicit Euler scheme to collect data of numerical experiments. They discretized the solution value for each cell and found local rules of a CA. As a test problem to discuss the validity of the experimental method, it is reasonable to consider applications to spatiotemporal data obtained by solving a PDE numerically. One may say the experimental method is valid if the resultant CA captures some properties of a target PDE. Kawaharada and Iima derived two kinds of CAs [3]: a deterministic CA and a stochastic CA. The former is a CA in which no randomness is involved, while the latter is a CA whose local rule is randomly chosen according to a given probability matrix at every time step. They applied their CA constructing method to a set of numerical solutions of the diffusion equation. Although the deterministic CA did not exhibit diffusion, it is manifested in the stochastic CA. Those results imply that CAs obtained by the experimental method may represent different behavior from those of the original datasets. Hence, it is important to investigate this statistical CA constructing procedure to evaluate its availability, and we shall consider its relevance to the original PDEs.

To discuss the relationship between a given PDE and a CA obtained by the experimental method, the manner of how the local rules are derived by the given PDE is an important point for consideration. However, the resultant CA by the experimental method is hardly identified a priori in a theoretical manner. For the theoretical study, the knowledge on how the distribution of values of the numerical solutions changes in time is important because the method is based on statistical treatment of numerical data whose distribution may vary in each step of the numerical calculation. It is a fact that even a linear combination of uniformly distributed random variables no longer obeys the uniform distribution [7]. Because the experimental method takes into account all arrangements of values of the adjacent cells over the whole experimental period, the distribution of the values of the adjacent cells may become complicated. We have not obtained a concrete theory that guarantees the validity of the CAs obtained by the experimental method. Therefore, we hardly recognize beforehand whether it is an appropriate mathematical model for the phenomenon under consideration.

Recently, according to the point related to the necessity of theoretical understanding of the choice of the local rules, Kawaharada, Miyaji, and Nakano proposed a different method of collecting data in numerical experiments [4]. The method is compatible with the theoretical study on the selectivity of the CA unlike with the experimental method. The key idea is to design a minimal set of numerical experiments to realize all possible combinations of states for adjacent three cells, which is called *the minimal method*. We can regard the minimal method as a simplified model of the experimental method (Figure 1), which focuses on the adjacent three cells instead of calculating the states of the cells in the whole space.

In the work obtained by Kawaharada, Miyaji, and Nakano [4], the minimal method was applied to the diffusion, the advection, and Burgers' equations. These equations were chosen in their work to check the availability of the method for these simple and basic equations, where they obtained consistent results with the experimental method. The dependence on the data set size was also studied in [4] using numerical experiments. The probability matrix of a stochastic CA obtained by the minimal method converges to the limit as the size of data set L tends to infinity and that the rate of convergence is approximately $1/\sqrt{L}$. On the other hand, the rule of a deterministic CA may vary, depending on the parameters of the corresponding difference equation. Hence, to overcome these difficulties, the robustness of the selectivity of the local rules must be considered.

This study aims to propose an approach to establish a theoretical foundation for the experimental method. We would like to obtain a theoretical understanding for the experimental method through the mathematical analysis of the minimal method. In particular, we consider two limit cases: (a) the number of states of CA goes to infinity and (b) the size of spatiotemporal data goes to infinity. In case (a), the CA obtained by the minimal method converges to the corresponding difference equation when the number of states of CA, which is the state resolution, goes to infinity. The convergence provides supporting evidence of the validity of the minimal and the experimental methods. Moreover, in case (b), we study the limit of the large number of spatiotemporal data to derive a condition that the local rule is uniquely determined in the cases of the diffusion and the advection equations. The uniqueness affects the robustness of the local rule obtained using the minimal method, which is important because the minimal method is a kind of Monte-Carlo method.

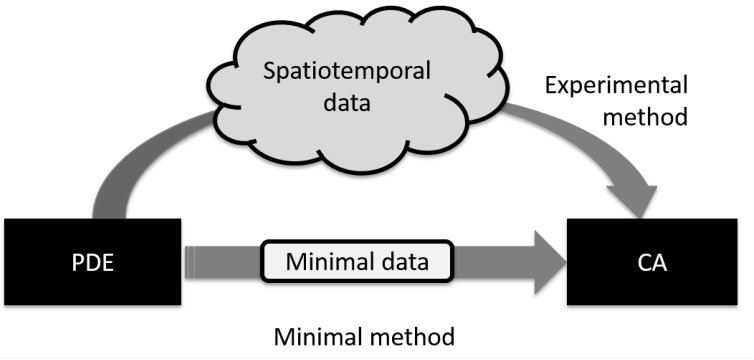


Figure 1: The relationship between the minimal method (analyzable method) and the experimental method.

This paper is organized as follows. The preliminaries on CAs, PDEs, and the experimental method of constructing a CA from a PDE are given in Section 2. We present the procedure of the minimal method in Section 3. In Section 4, we show our main results: mathematical analysis for the minimal method. In Section 5, we perform the construction of CAs using the minimal method for the diffusion, the advection, and Burgers' equations. Finally, we conclude in Section 6.

2 Preliminaries

2.1 Cellular automata

Two definitions are given for cellular automata. Let $A = \{0, 1, \ldots, k-1\}$ be a finite set with the cardinality $k = |A|$. The set of bi-infinite sequences of A is denoted by $A^{\mathbb{Z}}$, and it is called a *configuration space*, where $\mathbb{Z}$ is the set of all integers. An element $x = (x_i)_{i\in\mathbb{Z}} \in A^{\mathbb{Z}}$ is called a *configuration*, and x_i is called the *state* at the i-th cell. Since we regard A as a set of possible states, a configuration is an infinite collection of states distributed on the one-dimensional lattice $\mathbb{Z}$.

Definition 1. *Let f be a map from A^3 to A. Define a map T from $A^{\mathbb{Z}}$ to itself by $(Tx)_i = f(x_{i-1}, x_i, x_{i+1})$ for all $i \in \mathbb{Z}$. A cellular automaton (CA) is a dynamical system on $A^{\mathbb{Z}}$ equipped with evolution operators defined by iterations of T. Each correspondence from $(a, b, c) \in A^3$ to $d \in A$ is called a local rule of the CA.*

Definition 2. *Let $P = (p_{\alpha,l})$ be a $k^3 \times k$ probability matrix, that is, $\sum_{l=0}^{k-1} p_{\alpha,l} = 1$ and $0 \le p_{\alpha,l} \le 1$ hold for all $\alpha = 0, 1, \ldots, k^3 - 1$, where the indices begin with zero. A stochastic CA is a discrete-time stochastic process $x^0, x^1, \ldots, x^n, \ldots$ in $A^{\mathbb{Z}}$ such that for each $n, i \in \mathbb{Z}$, and $l \in A$, the probability that $x_i^{n+1} = l$ is $p_{\alpha,l}$, where $x^n = (x_i^n)_{i\in\mathbb{Z}}$ and $\alpha = k^2 x_{i-1}^n + k x_i^n + x_{i+1}^n$.*

We call a CA a deterministic CA to distinguish it from a stochastic CA.

2.2 Partial differential equations

We introduce three partial differential equations.

Definition 3. *The diffusion equation is defined by*

$$\frac{\partial u}{\partial t}(x,t) = \nu \frac{\partial^2 u}{\partial x^2}(x,t). \tag{2.1}$$

$u(x,t)$ is the density of the diffusing material at location $x \in \mathbb{R}$ and time $t \in \mathbb{R}$ $(t > 0)$, where $\mathbb{R}$ is the set of real numbers. The parameter ν denotes the diffusion coefficient.

For discretized space variable $x_i = i\Delta x$ and discretized time $t_n = n\Delta t$ let $u_i^n := u(x_i, t_n)$. We have the difference diffusion equation;

$$u_i^{n+1} = u_i^n + K(u_{i-1}^n + u_{i+1}^n - 2u_i^n), \tag{2.2}$$

where $K := \nu\Delta t/\Delta x^2$ $(\leq 1/2)$, called the *diffusion number*, is the only parameter. K should be less than $1/2$ so that the numerical scheme is stable. $K = 1/2$ is the threshold of the stability condition.

Figure 2(a) shows a space–time plot of a solution of (2.2) with $K = 0.4$, $i = 0, \ldots, 99$, and $n = 0, \ldots, 99$. We imposed the periodic boundary condition $u_0^n = u_{100}^n$ for all n and the initial condition

$$u_i^0 = \begin{cases} 1 & i = 48, \ldots, 52, \\ 0 & \text{otherwise.} \end{cases} \tag{2.3}$$

The solution of (2.2) gradually diffuses and eventually tends to a spatially homogeneous equilibrium. Larger K results in faster diffusion.

Definition 4. *The advection equation is defined by*

$$\frac{\partial u}{\partial t}(x,t) + c\frac{\partial u}{\partial x}(x,t) = 0. \tag{2.4}$$

The parameter $c > 0$ denotes the constant velocity of the advection.

A solution of the advection equation is continuous in both space and time, provided that the initial data is continuous. Discretizing the space and time variables, we obtain the difference advection equation

$$u_i^{n+1} = u_i^n - K(u_i^n - u_{i-1}^n) = (1-K)u_i^n + Ku_{i-1}^n \tag{2.5}$$

where $K := c\Delta t/\Delta x$ $(0 \leq K \leq 1)$. K should be equal or less than 1 so that the numerical scheme is stable.

Figures 3(a) and 4(a) show space–time plots of a solution of (2.5) with $K = 0.7$ and $K = 0.3$, respectively, where $i = 0, 1, \ldots, 99$, and $n = 0, 1, \ldots, 99$. We assigned the periodic boundary condition and the initial condition

$$u_i^0 = \begin{cases} 1 & i = 23 \ldots, 27, \\ 0 & \text{otherwise.} \end{cases} \tag{2.6}$$

Recall that the solution profile of (2.4) shifts to the right-hand side keeping its shape as time passes. In contrast, that of (2.5) behaves in a similar way, but its shape gradually deforms due to the numerical diffusion. Larger K leads to faster shift. The solutions do not move if $K = 0$, but they move at a constant velocity of 1 if $K = 1$.

Definition 5. *Burgers' equation is defined by*

$$\frac{\partial u}{\partial t}(x,t) + u(x,t)\frac{\partial u}{\partial x}(x,t) = \mu \frac{\partial^2 u}{\partial x^2}(x,t). \tag{2.7}$$

The parameter μ denotes the viscosity coefficient.

For discretized space and time we have the difference Burgers' equation;

$$u_i^{n+1} = u_i^n - K_1 u_i^n (u_i^n - u_{i-1}^n) + K_2 (u_{i+1}^n - 2u_i^n + u_{i-1}^n), \tag{2.8}$$

where $K_1 := \Delta t/\Delta x$, $K_2 := \mu \Delta t/\Delta x^2$. We assume $K_2 \leq 1/2$ and $K_1 \leq 1 - 2K_2$ for numerical stability.

Figure 5(a) shows a space–time plot of a solution of (2.8) with $K_1 = 0.7$, $K_2 = 0.14$, $i = 0, 1, \ldots, 149$, and $n = 0, 1, \ldots, 199$. We imposed the periodic boundary condition and the initial condition

$$u_i^0 = \begin{cases} 1 & i = 38 \ldots, 74, \\ 0 & \text{otherwise.} \end{cases} \tag{2.9}$$

The solution of (2.8) forms discontinuity in finite time, which is a so-called shock wave, which is a typical feature of Burgers' equation. The discontinuity propagates to the right-hand side of the shock wave, while the left-hand side is in a gradual decline.

2.3 Procedure of the experimental method

We recall the experimental method [2]. We consider the initial-boundary value problem of (2.2), (2.5), and (2.8) on a finite interval with the periodic boundary condition. In what follows, we suppose $0 \leq u_i^n \leq 1$ for all i and n. We discretize $u_i^n \in [0, 1]$ by

$$a = \mathrm{floor}(k u_i^n) \tag{2.10}$$

to regard a as a state of a CA, where $\mathrm{floor}(x)$ is the maximum integer less than or equal to x. As an exception, let $a = k - 1$ if $u_i^n = 1$. The restriction that $u_i^n \in [0, 1]$ is assumed for simplicity. The range of u_i^n can be arbitrary. In addition, inhomogeneous subintervals can be used to discretize states if needed (See [2]).

The experimental method is summarized as follows:

(1) Repeat the followings L times:

   (a) Generate random numbers $\{u_i^0\}_{0 \leq i < I}$ which obey the uniform distribution on $[0, 1]^I$.

   (b) Solve the difference equation until $n = N$ with the initial data $\{u_i^0\}_{0 \leq i < I}$.

   As a result, we obtain a dataset

$$\{u_{l,i,n} \mid 1 \leq l \leq L, 0 \leq i < I, 0 \leq n \leq N\},$$

   where $u_{l,i,n}$ denotes the solution value of the difference equation at position i and time n of the l-th trial.

(2) Convert $u_{l,i,n}$ to $a_{l,i,n}$ by

$$a_{l,i,n} = \mathrm{floor}(k\, u_{l,i,n})$$

   for all l, i, n.

(3) For each $a, b, c, d \in A$, let $X(a, b, c, d)$ be the number of combinations of elements in the dataset such that

$$(a_{l,i-1,n}, a_{l,i,n}, a_{l,i+1,n}, a_{l,i,n+1}) = (a, b, c, d),$$

   where i is taken modulo I.

(4) For each $(a, b, c) \in A^3$, find $d \in A$ which maximizes $X(a, b, c, d)$ and adopt the map $f(a, b, c) = d$ as a local rule of the CA.

For stochastic CAs, replace the final step by the following:

(4') For each $(a, b, c) \in A^3$, set

$$p_{\alpha,d} = \frac{X(a, b, c, d)}{\sum_{d \in A} X(a, b, c, d)},$$

   where α is the k-adic number of (a, b, c), that is, $\alpha = ak^2 + bk + c$.

3 Procedure of the minimal method

In this section, we introduce the minimal method [4], that is a modification of the experimental method. We represent a difference equation that approximates a given PDE by

$$u_i^{n+1} = H(u_{i-1}^n, u_i^n, u_{i+1}^n), \tag{3.1}$$

where $H : \mathbb{R}^3 \to \mathbb{R}$ is a corresponding continuous function to the explicit difference scheme of the numerical integration. For example, if the diffusion equation is given, we define

$$H(x, y, z) = y + K(x - 2y + z). \tag{3.2}$$

Again, for simplicity, we suppose $0 \leq u_i^n \leq 1$ for all i and n. It is easy to generalize the method to the case where the range of u_i^n is arbitrary.

The procedure of the minimal method is summarized as follows:

(1) For each $(a, b, c) \in A^3$, set $X(a, b, c, d) = 0$ and repeat the following procedure L times:

  (a) Pick a set of random numbers (x, y, z) which obeys the uniform distribution on

$$\left[\frac{a}{k}, \frac{a+1}{k}\right) \times \left[\frac{b}{k}, \frac{b+1}{k}\right) \times \left[\frac{c}{k}, \frac{c+1}{k}\right).$$

  (b) Compute $d = \mathrm{floor}(kH(x, y, z))$.

  (c) Increment $X(a, b, c, d)$.

(2) For each $(a, b, c) \in A^3$, find $d \in A$ which maximizes $X(a, b, c, d)$ and adopt the map $f(a, b, c) = d$ as a local rule of the CA.

A probability matrix of a stochastic CA is constructed by replacing Step (2) by Step (4') of the experimental method in the same manner.

4 Mathematical analysis of the minimal method

In this section, we mathematically analyze two ideal cases of the minimal method. First we consider the convergence of the CA constructed by the minimal method in the limit of large k. Next, we consider the uniqueness of the local rule of the the resultant CA obtained by the minimal method in the limit of large L. Before presenting the detailed analysis, let us note some basic facts. Let (a, b, c) be an arbitrary element of A^3 and D be the set

$$D = \left[\frac{a}{k}, \frac{a+1}{k}\right) \times \left[\frac{b}{k}, \frac{b+1}{k}\right) \times \left[\frac{c}{k}, \frac{c+1}{k}\right),$$

consisting of (x, y, z) whose states are given by (a, b, c). For any $(x, y, z) \in D$, $H(x, y, z)$ is contained in the interval

$$Y = H\left(\left[\frac{a}{k}, \frac{a+1}{k}\right), \left[\frac{b}{k}, \frac{b+1}{k}\right), \left[\frac{c}{k}, \frac{c+1}{k}\right)\right).$$

If (x, y, z) is a random variable obeying the uniform distribution on D, $w = H(x, y, z)$ is also a random variable following a certain distribution whose support is Y. Suppose an ideal case that we apply the minimal method with infinitely large L. Then the minimal method derives the local rule $f(a, b, c) = d$ so that $d \in A$ maximizes the probability $P(w \in Z_d)$, where

$$Z_d = Y \cap \left[\frac{d}{k}, \frac{d+1}{k}\right).$$

In the case that Z_d is empty for some $d \in A$, $f(a, b, c) = d$ cannot occur.

If the maximizer of $P(w \in Z_d)$ is not unique, then we cannot obtain a deterministic local rule for such $(a, b, c) \in A^3$ in a ideal situation $L = \infty$. In practice, the local rule for such (a, b, c) is quite sensitive to the dataset generated by pseudorandom numbers used in step 1 (a) of the procedure of the minimal method, because only the dataset of the trials of finite L can be used. To avoid this sensitivity of local rules, the appropriate system parameters need to be selected, for example, K in the difference diffusion equation. Let us say that a local rule is uniquely decidable if the maximizer is unique.

In this section, we denote the fractional part of a real number x by $\{x\}$. We will frequently use the following identity:

$$x = \mathrm{floor}(x) + \{x\}.$$

Obviously, we have $0 \leq \{x\} < 1$.

4.1 Convergence of local rules

In this section, we prove the following theorem.

Theorem 1. *Suppose that $H : \mathbb{R}^3 \to \mathbb{R}$ is a continuous function. For any $(u, v, w) \in [0, 1)^3$, let $(a, b, c) \in A^3$ be defined by*

$$a = \mathrm{floor}(ku), \quad b = \mathrm{floor}(kv), \quad c = \mathrm{floor}(kw). \tag{4.1}$$

Let $z = H(u, v, w)$ and f be the local rule of CA for H constructed by the minimal method. Then $f(a, b, c)/k \to z$ as k tends to infinity.

Proof. Let $\underline{z}, \overline{z}$ be given by

$$\underline{z} = \inf_{(u,v,w)\in D} H(u, v, w), \quad \overline{z} = \sup_{(u,v,w)\in D} H(u, v, w). \tag{4.2}$$

Let $\underline{r}, \overline{r}$ be defined by

$$\underline{r} = \mathrm{floor}(p\underline{z}), \quad \overline{r} = \mathrm{floor}(p\overline{z}), \tag{4.3}$$

where $p = 1/k$. Note that the candidates of the local rule for $(a, b, c) \in A$ is an integer contained in $[\underline{r}, \overline{r}]$. We have

$$p\underline{r} \ \leq \ \underline{z} \ \leq z \ \leq \ p\overline{r} \ \leq \ \overline{z}. \tag{4.4}$$

It is easy to see that

$$\begin{aligned} p\underline{r} &= p\ \mathrm{floor}(p^{-1}\underline{z}) = p(p^{-1}\underline{z} - \left\{p^{-1}\underline{z}\right\}) = \underline{z} - p\left\{p^{-1}\underline{z}\right\}, \\ p\overline{r} &= p\ \mathrm{floor}(p^{-1}\overline{z}) = p(p^{-1}\overline{z} - \left\{p^{-1}\overline{z}\right\}) = \overline{z} - p\left\{p^{-1}\overline{z}\right\}. \end{aligned}$$

The continuity of H implies that $\underline{z}$ and $\overline{z}$ converges to z as $k \to \infty$. Therefore we obtain

$$p\underline{r} \to z, \quad p\overline{r} \to z \tag{4.5}$$

as $k \to \infty$. By the squeeze theorem, $f(a, b, c)/k$ also tends to z. □

Corollary 1. *For difference advection equation, difference diffusion equation, and difference Burgers' equation, the local rule of a CA constructed by the minimal method converges to the difference equation as the number of states of CA goes to infinity.*

Consequently, this result implies that the difference equation can be regarded as a CA with an infinitesimal resolution of states.

4.2 Uniqueness of local rules

For the difference diffusion equation, we can prove the uniqueness of a local rule under a certain condition in the limit of large L. First, in the case of the diffusion equation, we prove that the candidates of the local rule for a given triplet $(a, b, c) \in A^3$ are just two.

Theorem 2. *Let a, b, and c be arbitrary elements in A. Let $(x, y, z) \in D = [a/k, (a+1)/k) \times [b/k, (b+1)/k) \times [c/k, (c+1)/k)$. For the difference diffusion equation, the discretization of $w = H(x, y, z)$ is either $r = \mathrm{floor}(kH(a/k, b/k, c/k))$ or $r + 1$.*

Proof. Since $1 - 2K > 0$, we have

$$H(D) = [H(pa, pb, pc), H(p(a+1), p(b+1), p(c+1)))\,, \tag{4.6}$$

where $p = 1/k$. Moreover, we obtain

$$\begin{aligned} H(pa, pb, pc) &= (1-2K)pb + K(pa + pc) \\ &= pH(a, b, c), \end{aligned}$$

and

$$\begin{aligned} H(p(a+1), p(b+1), p(c+1)) &= (1-2K)p(b+1) + K(p(a+1) + p(c+1)) \\ &= p\left[(1-2K)pb + K(pa + pc) + 1\right] \\ &= pH(a, b, c) + p. \end{aligned}$$

Since the width of the interval $H(D)$ is $p = 1/k$, the width of $kH(D)$ is unity. It implies that the discretization of $w = H(x, y, z)$ is either $r = \mathrm{floor}(kH(a/k, b/k, c/k))$ or $r + 1$. □

Next, we present a necessary condition that the local rule is not uniquely decidable.

Theorem 3. *Consider the difference diffusion equation. The local rule is not uniquely decidable only if K is representable by irreducible fraction $K = m/n$, where m is odd and n is even.*

Proof. Let $(a, b, c) \in A^3$ and $r = \mathrm{floor}(kH(pa, pb, pc))$. Since the density function of a linear combination of three uniform random variables is symmetric with respect to the mean value [7], we can compare the frequency by the Lebesgue measure instead of the probability measure. The local rule is not uniquely decidable if and only if $kH(pa, pb, pc) = r + 1/2$. In other words, the fractional part of $kH(pa, pb, pc)$ is $1/2$. It implies that the fractional part of $K(a - 2b + c)$ is $1/2$. Indeed, we have

$$kH(pa, pb, pc) = (1-2K)b + K(a + c) = b + K(a - 2b + c). \tag{4.7}$$

Since b is an integer, only $K(a - 2b + c)$ has a fractional part. Therefore, we obtain

$$K(a - 2b + c) - \mathrm{floor}(K(a - 2b + c)) = \frac{1}{2}. \tag{4.8}$$

It is equivalent to

$$K = \frac{2\mathrm{floor}(K(a - 2b + c)) + 1}{2(a - 2b + c)}. \tag{4.9}$$

Then K is representable by an irreducible fraction $K = m/n$, where m is odd and n is even. □

Notice that this theorem gives just a necessary condition. It is possible that the local rule is uniquely decidable even if K takes the form of odd/even. The contraposition of Theorem 3 gives a concrete criterion for the uniqueness.

Corollary 2. *If K in* (2.2) *satisfies one of the following three conditions, then the local rule of the resultant CA obtained by the minimal method is uniquely decidable.*

1. *K is irrational,*

2. K is an irreducible fraction of two odd numbers, or

3. K is an irreducible fraction m/n, where m is even and n is odd.

If $K = 0.4 = 2/5$, for example, then the local rule is uniquely decidable. Suppose $K = 0.5 = 1/2$ and $a = b$. In this case, we have

$$K(a - 2b + c) = \frac{c - b}{2}.$$

If b and c have opposite parity, then the fractional part of $K(a - 2b + c)$ is $1/2$, and hence the local rule for (a, b, c) is not uniquely decidable.

It should be noted that Theorems 2 and 3 and Corollary 1 are also valid for the difference advection equation with $0 < K < 1$. Indeed, the proofs are analogous if $H(x, y, z) = y + K(x - 2y + z)$ is replaced by $H(x, y, z) = y - K(y - x)$.

5 Numerical examples

In this section, we show space–time diagrams of CAs constructed from (2.2), (2.5), and (2.8) by the minimal method with $L = 10^3$. $L = 10^3$ is sufficiently large for constructing local rules of a deterministic CA as shown in [4]. Although a probability matrix of a stochastic CA changes depending on L, we obtained similar results for larger values of L. Section IV.B of [4] discussed the numerical study on how the resultant local rule of a CA depends on L. We used the Mersenne Twister to generate pseudorandom numbers [8].

5.1 Diffusion CAs

We applied the minimal method to (2.2) for all combination of $K = 0.1, 0.2, 0.3, 0.4, 0.5$ and $k = 2, 3, 4, 8$. For all cases, the initial configurations are $x_l = 0$ for all l except successive five cells on which $x_l = k - 1$, and the periodic boundary conditions are imposed. All results are qualitatively similar to succeeding explanation. Figure 2(b) shows the space–time diagram of deterministic CA for $K = 0.4$. Figure 2(c) shows the average of 1000 samples of stochastic CA.

Comparing the results with Figure 2(a), the deterministic CA's diagram is diffusive only for a short period of time, and it settles into a static state. On the other hand, the stochastic CA's diagram shows diffusive behavior for a long time. When K is small, the diffusion width is small. The width increases monotonically as K tends to 0.5. These are consistent with the results by [2].

(a) Difference eq. (b) Deterministic CA (c) Stochastic CA

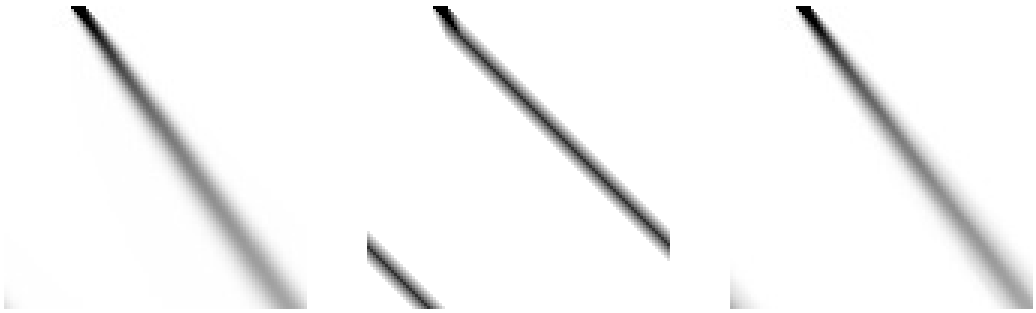
Figure 2: (a) Space–time plot of (2.2) with $K = 0.4$, $i = 0, \ldots, 99$, and $n = 0, \ldots, 99$. The initial condition is given by 1 for $i = 48, \ldots, 52$; 0 otherwise. The periodic boundary condition is applied. (b) Space–time diagram of deterministic diffusion CA for $K = 0.4$ with possible states $k = 8$. (c) Average of 1000 space–time diagrams of stochastic diffusion CA for $K = 0.4$ with possible states $k = 8$. (For (b) and (c), their initial configurations are given by five site seeds and the periodic boundary condition is applied (space size: 100, time steps: 100).)

5.2 Advection CAs

We applied the minimal method to (2.5) for all combinations of $K = 0.1$, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0 and $k = 2, 3, 4, 8$. The initial and boundary conditions are similar with those of (2.2). Figures 3 and 4 show space–time diagrams of advection CAs with $k = 8$ for $K = 0.7$ and $K = 0.3$, respectively.

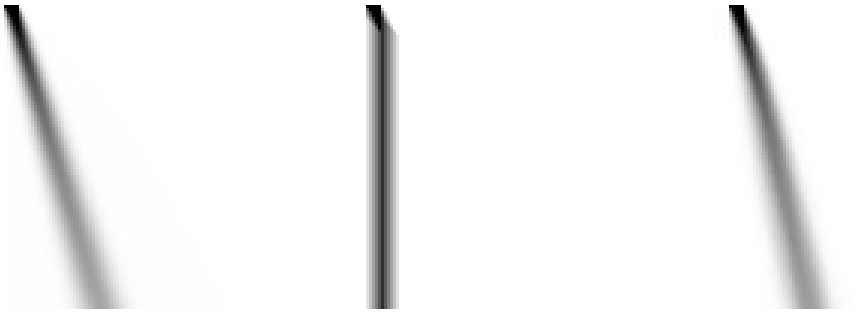
For the deterministic case, $K = 0.5$ is the threshold at which the feature of diagrams drastically changes. When K is greater than 0.5, e.g., $K = 0.7$ in Figure 3, we can observe the advection at the constant velocity 1. On the other hand, when K is smaller than 0.5, e.g., $K = 0.3$ in Figure 4, although it looks like a vertical line at a glance, nonzero states move only a few steps and settle into a static state. For the stochastic cases, we can observe the advective behavior at the same velocity as a solution of (2.5).

Note that both $K = 0.3$ and $K = 0.7$ are the cases where the local rule of the deterministic CA is not uniquely decidable. For example, even if we take large L, $f(7, 2, 0)$ can be either 3 or 4 depending on L and the seed of pseudorandom numbers in the case of $K = 0.3$. In fact, we applied the minimal method ten times, and we obtained ten different local rules. Nevertheless, similar space–time diagrams were obtained even though the local rules were different. The difference of local rules did not significantly affect the dynamics in this example.



(a) Difference eq. (b) Deterministic CA (c) Stochastic CA

Figure 3: (a) Space–time plot of (2.5) with $K = 0.7$, $i = 0, \ldots, 99$, and $n = 0, \ldots, 99$. The periodic boundary condition is applied. (b) Space–time diagram of deterministic advection CA for $K = 0.7$, $k = 8$. (c) Average of 1000 space–time diagrams of stochastic advection CA for $K = 0.7$, $k = 8$. (For (b) and (c), their initial configurations are given by five site seeds and the periodic boundary condition is applied. (space size: 100, time steps: 100).)

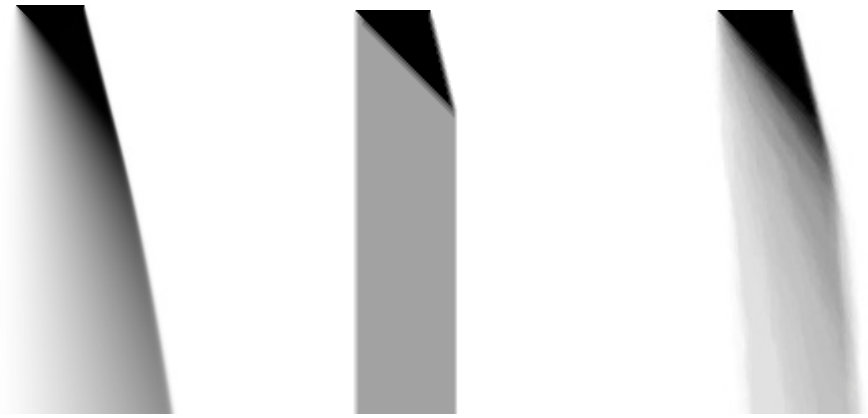


(a) Difference eq. (b) Deterministic CA (c) Stochastic CA

Figure 4: (a) Space–time plot of (2.5) with $K = 0.3$, $i = 0, \ldots, 99$, and $n = 0, \ldots, 99$. The periodic boundary condition is applied. (b) Space–time diagram of deterministic advection CA for $K = 0.3$, $k = 8$. (c) Average of 1000 space–time diagrams of stochastic advection CA for $K = 0.3$, $k = 8$. (For (b) and (c), their initial configurations are given by five site seeds and the periodic boundary condition is applied. (space size: 100, time steps: 100).)

5.3 Burgers' CAs

We applied the minimal method to (2.8) with $(K_1, K_2) = (0.7, 0.14)$ for $k = 2, 3, 4, 8$. We imposed the periodic boundary condition, and the initial configuration was zero for all i except $38 \leq i < 75$ for which the state is $k-1$. We obtained qualitatively similar results for all $k = 2$, 3, 4, 8. Figure 5(b) shows the space–time diagram of the deterministic CA with $k = 8$. Figure 5(c) shows an average of 1000 space–time diagrams of stochastic CA with $k = 8$. Comparing these figures with Figure 5(a), we found that the deterministic CAs with $|A| \leq 8$ can reproduce neither advection (the right-side) nor dissipation (the left-side). On the other hand, because the stochastic CAs can reproduce both, Figure 5(a) and Figure 5(c) are similar.



(a) Difference eq. (b) Deterministic CA (c) Stochastic CA

Figure 5: (a) Space–time plot of (2.8) with $K_1 = 0.7$, $K_2 = 0.14$, $i = 0, \ldots, 149$, and $n = 0, \ldots, 199$. The initial condition is given by 1 for $i = 38, \ldots, 74$; 0 otherwise. The periodic boundary condition is applied. (b) Space–time diagram of deterministic Burgers' CA for $K_1 = 0.7$, $K_2 = 0.14$ with $k = 8$. (c) Average of 1000 space–time diagrams of stochastic Burgers' CA for $K_1 = 0.7$, $K_2 = 0.14$ with $k = 8$. (For (b) and (c), their initial configurations are given by $k - 1$ if $38 \leq i < 75$; 0 otherwise, and the periodic boundary condition is applied (space size: 150, time steps: 200).)

6 Discussion and concluding remarks

The minimal method was proposed as a simplified model of the experimental method, applied to datasets of numerical solution of PDEs to examine the selectivity of the local rules [4]. It produces consistent results with the experimental method as is shown in [4]. In this study, we have shown its selectivity and robustness by mathematical analysis. The results are as follows.

In Theorem 2, we have proved that we have at most two candidates of the local rule for any given triplet $(a, b, c) \in A^3$ for the diffusion and the advection equations. In Theorem 3 and Corollary 2, we have derived conditions that the minimal method gives a robust result for the difference diffusion equation. The analysis in Section 4.2 can be applied to Burgers' equation. Since Burgers' equation is nonlinear, the situation may become more complicated. For example, there can be more than two candidates of the local rule. Therefore, a more careful analysis is needed for Burgers' equation and we postpone it to future work.

As the number of states increases, by Theorem 1, the resultant CA of the minimal method tends to the difference equation which is a numerical scheme of a given PDE. In this sense, the minimal and the experimental methods are closely related to the difference equation. This suggests that these methods can be an approach to Wolfram's 9th problem, which asks the correspondence between CAs and PDEs [10]. This problem encouraged the development of the ultra-discretization method and led to successful linking of CAs and PDEs, especially integrable PDEs [9, 1]. The ultra-discretization and its inverse could be a reliable approach to convert between a PDE and a CA. It is, however, hard

to apply the method to non-integrable PDEs. Although there are some successful examples, it is too technical for non-professionals. On the other hand, the minimal and the experimental methods have an advantage that it is applicable to any dynamical system in principle.

Theorem 1 provides a partial answer to the validity of the experimental method from the viewpoint of numerical analysis. Note that we cannot conclude that a small k gives a wrong CA as a model of a PDE , because k corresponds to the resolution of states of a CA. (Actually, $1/k$ denotes a resolution.) In other words, each CA with k contains dynamical information corresponding to each resolution. If some CA shows different behavior from the original PDE, then the resolution in that case is too crude. Moreover, in a practical point of view, one cannot take k so large because of the memory limitation. In addition, a CA has an advantage that it can generate rich spatiotemporal patterns even if k is small. Therefore, it is interesting to note the case of small k.

In Section 5, we have shown numerical examples for three differential equations. Advection and diffusion may be important elements of more complicated phenomenon. Burgers' equation is a nonlinear example that possesses both characteristics of advection and diffusion. The previous studies supposed the number of states is less than or equal to eight ([4], [5], [2], [6], and [3]), and we have used $k = 8$ in this study, which is far from the limit $k \to \infty$. Nevertheless, a stochastic CA obtained by the minimal method reproduces qualitative feature of the corresponding difference equation in each case.

Recall that the exact solution of the advection equation shifts to the right-hand side keeping its profile, while the difference advection equation (2.5) exhibits numerical diffusion and the solution profile is gradually deformed. As shown in Figure 3, the stochastic CA captures such numerical diffusion, *viz.*, the stochastic CA may capture and reproduce such characteristics caused by the numerical integration scheme. On the other hand, the deterministic CA keeps the solution profile. Interestingly, it reproduces the advective behavior of the advection equation (2.4) rather than the difference equation (2.5).

We have seen that a deterministic CA does not necessarily give a good agreement with the difference equation. For the diffusion and Burgers' equations, the configuration of the deterministic CA immediately falls into a static state. This fact occurs from a defect in the resolution. To overcome this difficulty, it is important to choose proper resolutions of space, time, and state variables as shown in the work studied by Kawaharada, Miyaji, and Nakano [5]. Further studies to establish the theoretical background of the proper choice of the resolutions are needed. Our analysis in this study can be a theoretical basis for empirical CA construction methods that will be further developed in the future.

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