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Staggered Invariants in Cellular Automata

Shinji Takesue*
Department of Fundamental Sciences,
Faculty of Integrated Human Studies,
Kyoto University, Kyoto, 606–01, Japan

Abstract. A necessary and sufficient condition for a given cellular automaton (CA) rule to admit a *staggered* invariant is derived. This condition is written in the form of the equation of continuity. By utilizing the condition, a number of invariants are obtained in Wolfram's elementary CA and their reversible variants.

1. Introduction

Conserved quantities are one of the most fundamental characteristics of a dynamical system. In some cases, they are connected with symmetries of the system via Noether's theorem [1]. However, it is a difficult problem to find *all* conserved quantities for a given dynamical system. To find a set of conserved quantities, it is necessary to impose some restrictions on the properties of the conserved quantities.

For one-dimensional cellular automata (CA) with the periodic boundary condition of period N, a general method is given in [2] for finding *additive* conserved quantities of the form

$$\Phi(\mathbf{x}^t) = \sum_{l=0}^{N-1} F(x_l^t, x_{l+1}^t, \ldots, x_{l+\alpha}^t), \tag{1.1}$$

where $\mathbf{x}^t = (x_0^t, \ldots, x_{N-1}^t) \in X^N$ denotes dynamical variables, the set of site values X is arbitrary, and α is a given integer. In particular, for a time evolution rule of the form

$$x_l^{t+1} = g(x_{l-1}^t, x_l^t, x_{l+1}^t) \tag{1.2}$$

(i.e., the case of nearest-neighbor interactions), a necessary and sufficient condition for $\Phi(\mathbf{x}^t)$ to be constant is that the function F satisfies the equation of continuity

$$\begin{aligned} &G(x_0, x_1, \ldots, x_{\alpha+1}, x_{\alpha+2}) \\ &\quad = F(x_1, x_2, \ldots, x_{\alpha+1}) + J(x_0, x_1, \ldots, x_{\alpha+1}) - J(x_1, x_2, \ldots, x_{\alpha+2}), \end{aligned} \tag{1.3}$$

*Electronic mail address: takesue@phys.h.kyoto-u.ac.jp.

where function $G : X^{\alpha+3} \to \mathbf{R}$ is defined by

$$G(x_0, x_1, \ldots, x_{\alpha+2}) = F(g(x_0, x_1, x_2), g(x_1, x_2, x_3), \ldots, g(x_\alpha, x_{\alpha+1}, x_{\alpha+2})), \tag{1.4}$$

and the function $J : X^{\alpha+2} \to \mathbf{R}$ is defined by

$$J(x_0, x_1, \ldots, x_\alpha, x_{\alpha+1}) = \sum_{l=0}^{\alpha+1} \left[F(\overbrace{P, \ldots, P}^{\alpha+1-l}, x_0, x_1, \ldots, x_{l-1}) - G(\overbrace{P, \ldots, P}^{\alpha+2-l}, x_0, x_1, \ldots, x_l) \right] \tag{1.5}$$

with an arbitrary fixed value $P \in X$. If a CA rule and nonnegative integer α are specified, one can obtain, if any, all the functions F with which $\Phi(\mathbf{x}^t)$ is invariant by solving equation (1.3). In [2] the additive conserved quantities of range $\alpha \leq 6$ for elementary cellular automata (ECA) [3] and those of range $\alpha \leq 2$ for the elementary reversible cellular automata (ERCA) [4] are obtained. In the latter case, the additive conserved quantities are of particular importance for the statistical properties of the systems, because they can be considered as Hamiltonians in the sense of statistical mechanics.

Modeling a physical phenomenon with CA usually takes the converse approach. Namely, one looks for a rule that satisfies prescribed conservation laws. For example, lattice-gas automata for simulating fluid motions are devised to conserve the total number of particles and the total momentum.

There are cases where such models unexpectedly admit the existence of spurious invariants. The two-dimensional lattice-gas automata in [5] conserved total momenta on each line. The model was improved in [6] by using the triangular lattice instead of the square lattice. The model in [6] had been believed not to have conserved quantities other than the total number of particles and the total momentum. However, in [7] are found extra nonphysical invariants written as

$$H_\gamma = (-1)^t \sum_{\mathbf{r}} (-1)^{\mathbf{B}_\gamma \cdot \mathbf{r}} \mathbf{C}_\gamma^\perp \cdot \mathbf{g}(\mathbf{r}, t) \tag{1.6}$$

where $\mathbf{r}$ denotes a lattice point, $\mathbf{C}_\gamma^\perp$ ($\gamma = 1, 2, 3$) is a unit vector perpendicular to one of the three nonparallel lattice vectors of the triangular lattice, and $\mathbf{B}_\gamma = 2\mathbf{C}_\gamma/3$, and $\mathbf{g}(\mathbf{r}, t)$ is the momentum density. Since these invariants include factors $(-1)^t$ and $(-1)^{\mathbf{B}_\gamma \cdot \mathbf{r}}$, they are called *staggered* invariants. Staggered invariants are also found in other models of lattice-gas automata (e.g., [8, 9, 10]).

Thus, the staggered invariants were found and discussed for some lattice-gas automata, but there has been little discussion about them for more general CA. Since lattice-gas automata are a special kind of CA, some new interesting features may appear in general CA. For example, although staggered invariants found so far in lattice-gas automata are limited to the *linear* case, or $\alpha = 0$ in the present notation, those with $\alpha > 0$ are commonly seen in general CA. In this paper, the method of [2] is extended to give a general method of finding staggered invariants in one-dimensional CA and apply it to ECA and ERCA.

2. Conservation condition

Because the extension to general one-dimensional CA is straightforward, I concentrate on the case of nearest-neighbor interaction rules of the form (1.2). Let us consider quantities written as

$$\Psi(\mathbf{x}^t) = e^{\frac{2\pi i t}{\tau}} \sum_{l=0}^{N-1} e^{\frac{2\pi i l}{\lambda}} F(x_l^t, x_{l+1}^t, \ldots, x_{l+\alpha}^t) \tag{2.1}$$

under the periodic boundary condition of period N and assume that N is a multiple of λ. Given a rule g and integers α, τ, and λ, if this quantity is conserved for any N and any initial conditions, it is called a staggered invariant of range α and of type (τ, λ). Staggered invariants of type $(\tau, \lambda) = (1, 1)$ amount to additive conserved quantities.

In the following, a condition for Ψ to be invariant is derived in the same manner as in [2]. Clearly, if identity $\Psi(\mathbf{x}^{t+1}) = \Psi(\mathbf{x}^t)$ holds true at $t = 0$ for any initial condition $\mathbf{x}^0$, it remains true also for all $t > 0$. Representing $\mathbf{x}^0 = (x_0^0, x_1^0, \ldots, x_{N-1}^0)$ as $\mathbf{x} = (x_0, x_1, \ldots, x_{N-1})$ and using G defined by equation (1.4), one can write

$$\Psi(\mathbf{x}^1) = e^{\frac{2\pi i}{\tau}} \sum_{l=0}^{N-1} e^{\frac{2\pi i l}{\lambda}} G(x_{l-1}, x_l, \ldots, x_{l+\alpha+1}). \tag{2.2}$$

Hence, if Ψ is invariant, function $H(\mathbf{x})$ defined by

$$H(\mathbf{x}) \equiv \sum_{l=0}^{N-1} e^{\frac{2\pi i l}{\lambda}} \left[e^{\frac{2\pi i}{\tau}} G(x_{l-1}, x_l, \ldots, x_{l+\alpha+1}) - F(x_l, x_{l+1}, \ldots, x_{l+\alpha}) \right] \tag{2.3}$$

identically vanishes. Accordingly, inserting a particular value P into x_0 does not change the value of H. Thus one has

$$H(x_0, x_1, \ldots, x_{N-1}) - H(P, x_1, \ldots, x_{N-1}) = 0 \tag{2.4}$$

Substitution of equation (2.3) into equation (2.4) makes the Gs and Fs not including x_0 in their arguments cancel and leads to an identity composed of $2\alpha + 5$ variables $x_{N-\alpha-2}$, $x_{N-\alpha-1}, \ldots, x_{N-1}$, x_0, x_1, $x_2, \ldots, x_{\alpha+2}$. Since all these variables are arbitrary, one can insert value P into $x_{N-\alpha-2}, \ldots, x_N$ to obtain

$$\begin{aligned}
& e^{\frac{2\pi i}{\tau}} G(x_0, x_1, \ldots, x_{\alpha+2}) - F(x_1, x_2, \ldots, x_{\alpha+1}) \\
&\quad = -\sum_{l=0}^{\alpha+1} e^{-\frac{2\pi i (l+1)}{\lambda}} \Bigg[e^{\frac{2\pi i}{\tau}} G(\overbrace{P, \ldots, P}^{l+1}, x_0, \ldots, x_{\alpha+1-l}) \\
&\qquad - F(\overbrace{P, \ldots, P}^{l}, x_0, \ldots, x_{\alpha-l}) \Bigg] \\
&\qquad + \sum_{l=0}^{\alpha+1} e^{-\frac{2\pi i l}{\lambda}} \Bigg[e^{\frac{2\pi i}{\tau}} G(\overbrace{P, \ldots, P}^{l+1}, x_1, \ldots, x_{\alpha+2-l})
\end{aligned}$$

$$
\left. -F(\overbrace{P,\ldots,P}^{l},x_1,\ldots,x_{\alpha+1-l})\right]
$$

$$
+e^{-\frac{2\pi i(\alpha+2)}{\lambda}}\left[e^{\frac{2\pi i}{\tau}}G(P,\ldots,P)-F(P,\ldots,P)\right]. \tag{2.5}
$$

When $\lambda=1$, identity $H(P,\ldots,P)=0$ brings a further condition

$$
e^{\frac{2\pi i}{\tau}}G(P,P,\ldots,P)=F(P,P,\ldots,P), \tag{2.6}
$$

and the last term of the right-hand side of equation (2.5) vanishes. For the case when $\lambda\neq 1$, $H(P,\ldots,P)$ trivially vanishes and no new conditions appear.

Thus, if one defines the conserved current J as

$$
J(x_0,x_1,\ldots,x_{\alpha+1})=c(\tau,\lambda)+\sum_{l=0}^{\alpha+1}e^{-\frac{2\pi i(l+1)}{\lambda}}\left[F(\overbrace{P,\ldots,P}^{l},x_0,\ldots,x_{\alpha-l})\right.
$$

$$
\left.-e^{\frac{2\pi i}{\tau}}G(\overbrace{P,\ldots,P}^{l+1},x_0,\ldots,x_{\alpha+1-l})\right] \tag{2.7}
$$

where $c(\tau,\lambda)$ is defined by

$$
c(\tau,\lambda)=\begin{cases}0 & \text{for } \lambda=1,\\ \dfrac{e^{-\frac{2\pi i(\alpha+2)}{\lambda}}}{1-e^{\frac{2\pi i}{\lambda}}}\left[e^{\frac{2\pi i}{\tau}}G(P,\ldots,P)-F(P,\ldots,P)\right] & \text{otherwise.}\end{cases} \tag{2.8}
$$

Condition (2.5), incorporated with equation (2.6) in the case when $\lambda=1$, is rewritten into the form of the equation of continuity

$$
\begin{aligned}
&e^{\frac{2\pi i}{\tau}}G(x_0,x_1,\ldots,x_{\alpha+2})-F(x_1,x_2,\ldots,x_{\alpha+1})\\
&\quad=J(x_0,x_1,\ldots,x_{\alpha+1})-e^{\frac{2\pi i}{\lambda}}J(x_1,x_2,\ldots,x_{\alpha+2}).
\end{aligned} \tag{2.9}
$$

This is the conservation condition for Ψ.

Because the above condition was derived based on the assumption that Ψ is an invariant, it is a necessary condition. Conversely, it is obvious that if the condition is satisfied, Ψ is an invariant. Thus it is also a sufficient condition. Substitution of $(\tau,\lambda)=(1,1)$ into equations (2.7) and (2.9) reduces them to the condition for additive conserved quantities (1.3) and the definition of the conserved current in that case (1.5).

Here are a few remarks on the condition obtained in the preceding. First, the conserved density F is not uniquely determined for a staggered invariant Ψ. For a given F and an arbitrary function $S:X^\alpha\to\mathbf{R}$, function F' defined by

$$
F'(x_0,\ldots,x_\alpha)=F(x_0,\ldots,x_\alpha)+S(x_0,\ldots,x_{\alpha-1})-e^{\frac{2\pi i}{\lambda}}S(x_1,\ldots,x_\alpha) \tag{2.10}
$$

becomes a different density function for the same additive invariant Ψ. The difference between F and F' is called *surface terms.* To remove this arbitrariness, one may impose the condition

$$F(P, x_1, \ldots, x_\alpha) = F(P, P, \ldots, P). \tag{2.11}$$

This restriction somewhat simplifies the conservation condition as

$$\begin{aligned} &G(x_0, x_1, \ldots, x_{\alpha+2}) - e^{-\frac{2\pi i}{\lambda}} e^{-\frac{2\pi i}{\tau}} F(x_0, x_1, \ldots, x_\alpha) \\ &= \sum_{l=0}^{\alpha+1} e^{-\frac{2\pi i l}{\lambda}} \Bigg[G(\overbrace{P, \ldots, P}^{l+1}, x_1, \ldots, x_{\alpha+2-l}) \\ &\qquad - e^{-\frac{2\pi i}{\lambda}} G(\overbrace{P, \ldots, P}^{l+1}, x_0, \ldots, x_{\alpha+1-l}) \Bigg] \\ &\quad + \left[e^{-\frac{2\pi i(\alpha+2)}{\lambda}} G(P, \ldots, P) - e^{-\frac{2\pi i}{\tau}} e^{-\frac{2\pi i}{\lambda}} F(P, \ldots, P) \right] \end{aligned} \tag{2.12}$$

Note that the last term in the right-hand side vanishes when $\lambda = 1$. Also note that if either $\tau = 1$ or $\lambda \neq 1$, then $F(P, \ldots, P)$ can be set as zero, because a constant term generates a trivial invariant in the former case, or it is a kind of surface term in the latter case.

Second, the conserved density F itself may be periodic in time with period τ. If one can make a current J associated with F identically vanish by choosing the surface terms properly, such a function F is called a *localized periodic function.* This is the case when the set of $(\alpha + 1)$-site values $X^{\alpha+1}$ is divided into subsets as

$$X^{\alpha+1} = \bigcup_l B_l \tag{2.13}$$

with subsets B_k satisfying

$$B_l \cap B_k = \phi \quad \text{if} \quad l \neq k,$$

$$\begin{aligned} g^\tau(B_k) \equiv \{&(x_0^\tau, \ldots, x_\alpha^\tau) \in X^{\alpha+1} | (x_0^0, \ldots, x_\alpha^0) \in B_k, \\ &x_i^0 \in X \text{ for } i < 0 \text{ or } i > \alpha\} \\ \subset B_k &\text{ for } \forall k. \end{aligned}$$

If this condition is satisfied, the characteristic functions of subsets B_k,

$$\chi_k(b) = \begin{cases} 1 & \text{if } b \in B_k, \\ 0 & \text{otherwise} \end{cases} \tag{2.14}$$

become localized periodic functions. If there exists a localized periodic function of period τ, it is a conserved density of a staggered invariant of type (τ, λ) for an arbitrary λ at the same time.

3. Elementary cellular automata

The ECA in [3] are the simplest example of dynamics of the form (1.2), where set $X = \{0, 1\}$. Each rule is referred to by the number

$$\sum_{a=0}^{1}\sum_{b=0}^{1}\sum_{c=0}^{1} g(a,b,c)2^{4a+2b+c} \tag{3.1}$$

and there are 256 rules from rule 0 to rule 255 in ECA. However, reflection and boolean conjugation symmetries classify the 256 rules into 88 equivalence classes. This paper considers the 88 rules each of which has the smallest rule number in its class.

Given α, density function F can generally be represented with $2^\alpha + 1$ parameters $\{b_0, \ldots, b_{2^\alpha}\}$ as

$$\begin{aligned} F(x_0, x_1, \ldots, x_\alpha) &= b_0 + b_1x_0 + b_2x_0x_1 + b_3x_0x_2 + b_4x_0x_1x_2 + \cdots \\ &= b_0 + \sum_{(a_1,\ldots,a_\alpha)\in\{0,1\}^\alpha} b_k x_0 x_1^{a_1} \ldots x_\alpha^{a_\alpha} \end{aligned} \tag{3.2}$$

where $1 \le k \le 2^\alpha$ denotes the integer corresponding to the binary sequence $(a_1, \ldots, a_\alpha)$ through the relation

$$k = 1 + \sum_{i=1}^{\alpha} a_i 2^{i-1}. \tag{3.3}$$

Here the condition (2.11) is used with $P = 0$. If $\tau = 1$ or $\lambda \neq 1$, b_0 can be set as zero without loss of generality because it produces a trivial invariant or its sum vanishes identically, as remarked earlier.

Inserting equation (3.2) into the conservation condition (2.12), a set of linear and homogeneous equations for parameters $\{b_k\}$ is obtained. For example, when $\alpha = 1$, the equations are written as

$$C_1(x_0, x_1, x_2)b_1 + C_2(x_0, x_1, x_2)b_2 = 0 \tag{3.4}$$

where

$$\begin{aligned} C_1(x_0, x_1, x_2) = {} & g(x_0, x_1, x_2) - g(0, x_1, x_2) \\ & + e^{-\frac{2\pi i}{\lambda}}[g(0, x_0, x_1) - g(0, 0, x_1) - x_0 e^{-\frac{2\pi i}{\tau}}] \\ & + e^{-\frac{4\pi i}{\lambda}}[g(0, 0, x_0) - g(0, 0, 0)] \end{aligned} \tag{3.5}$$

and

$$\begin{aligned} C_2(x_0, x_1, x_2) = {} & g(x_1, x_2, x_3)[g(x_0, x_1, x_2) - g(0, x_1, x_2)] \\ & + e^{-\frac{2\pi i}{\lambda}}[g(0, x_0, x_1)g(x_0, x_1, x_2) - g(0, 0, x_1)g(0, x_1, x_2) - x_0x_1e^{-\frac{2\pi i}{\tau}}] \\ & + e^{-\frac{4\pi i}{\lambda}}[g(0, 0, x_0)g(0, x_0, x_1) - g(0, 0, 0)g(0, 0, x_1)] \\ & + e^{-\frac{6\pi i}{\lambda}} g(0, 0, 0)[g(0, 0, x_0) - g(0, 0, 0)]. \end{aligned} \tag{3.6}$$

Equation (3.5) must be satisfied for any values of (x_0, x_1, x_2). When both $\lambda \neq 1$ and $\tau = 1$ are satisfied, a further condition

$$b_0(1 - e^{-\frac{2\pi i}{\tau}}) + (b_1 + b_2)g(0,0,0) = 0 \tag{3.7}$$

is required. Similar equations are also obtained for a larger α, though their expressions are then more complicated.

The equations have been solved with the aid of computers in cases $(\tau, \lambda) = (1,1)$, $(1,2)$, $(2,1)$, and $(2,2)$ with $\alpha \leq 6$ for the 88 rules considered. Table 1 shows the number of staggered invariants of range $\alpha = 6$ for the 88 rules, where each number denotes the linear dimension of the solution space $\{b_i\}$, that is, the number of free parameters. Tables 2 through 4 show the staggered invariants of types $(\tau, \lambda) = (1,2)$, $(2,1)$, and $(2,2)$ up to range $\alpha = 4$. Additive conserved quantities of ECA for the same range α are found in [2].

As can be seen in Tables 1 through 4, the appearance of staggered invariants is always accompanied with some additive conserved quantities (i.e., $(\tau, \lambda) = (1,1)$). Moreover, the rules possessing staggered invariants belong to the class 2 according to the classifications in [11]. Namely, these rules develop space-time patterns consisting of separated periodic regions. Actually, the density functions of staggered invariants F correspond to these periodic patterns. For example, rule 12 conserves pattern $(x_i, x_{i+1}) = (0,1)$. Thus, $F(x_i, x_{i+1}) = (1 - x_i)x_{i+1}$ is a localized periodic function of period 1 and leads to a staggered invariant of type $(1,2)$ as well as an additive conserved quantity. Another example is rule 170, which works as a shift. Every pattern goes to the left by one site at a time step. Thus, any function is a density function of a staggered invariant of types $(1,1)$ and $(2,2)$. Other cases also have similar structures to these two examples.

Although the staggered invariants are connected with patterns generated by class-2 rules, not all class-2 rules have additive or staggered invariants. This is because contrary to the classifications in [3], which relates to asymptotic behavior of a system, the definition of invariants here is concerned with a property valid for all time t. Since ECA are dissipative systems, the condition for $\Psi(\mathbf{x}^{t+1}) = \Psi(\mathbf{x}^t)$ with $t > 0$ can be different from that for $\Psi(\mathbf{x}^1) = \Psi(\mathbf{x}^0)$. To obtain a better correspondence between patterns and invariant quantities, asymptotic properties must be considered. For example, in rule 104, pattern $(0,0,1,1,0,0)$ can be created from other patterns but cannot be destroyed if once created. Hence, the lattice sum of local values of its characteristic function approaches a constant in $t \to \infty$. The asymptotic behavior or the structure of attractors in an ECA should be well reflected by such asymptotic invariants. However, it is beyond the scope of the present paper.

Table 1: Number of staggered invariants of range $\alpha = 6$ for ECA.

Rule	Type (τ, λ)				Rule	Type (τ, λ)			
	$(1,1)$	$(1,2)$	$(2,1)$	$(2,2)$		$(1,1)$	$(1,2)$	$(2,1)$	$(2,2)$
0					**56**	1			
1	2	2	2	2	**57**				
2	3			3	**58**				
3	7		7		**60**				
4	5	5			**62**				
5	4	4	3	3	**72**	2	2		
6					**73**				
7					**74**				
8					**76**	18	18		
9					**77**	2	2		
10	6			6	**78**				
11	1				**90**				
12	8	8			**94**				
13					**104**				
14	1				**105**				
15	32	32	32	32	**106**				
18					**108**	5	5	1	1
19	1	1	1	1	**110**				
22					**122**				
23	1	1	1	1	**126**				
24	1			1	**128**				
25					**130**				
26					**132**	3	3		
27	4		4		**134**				
28					**136**				
29	5	5	5	5	**138**	9			9
30					**140**	8	8		
32					**142**	1			
33					**146**				
34	8			8	**150**				
35	1				**152**				
36	1	1			**154**				
37					**156**				
38	2	2	2	2	**160**				
40					**162**				
41					**164**				
42	20			20	**168**				
43	1				**170**	64			64
44					**172**	3	3		
45					**178**	1	1	1	1
46	2			2	**184**	1			
50	1	1	1	1	**200**	16	16		
51	32	32	32	32	**204**	64	64		
54					**232**	2	2		

Table 2: Staggered invariants of type $(1,2)$ up to range $\alpha = 4$ for ECA.

Rule	b_1	b_2	b_3	b_4	b_5	b_6	b_7	b_8	b_9	b_{10}	b_{11}	b_{12}	b_{13}	b_{14}	b_{15}	b_{16}
1	1		−1	1												
4	1			−1												
	1		−1			−1	1							1		−1
5	3		−1						1		−1					
	1			−1					1	−1	−1	1	−1	1	1	−1
12	1	1														
			1	−1		1		−1								
					1		−1			1				−1		
15	1															
			1	−2												
		1			1	−1	−1									
			1			1	−1									
		1			−1						2	−2	−2	−3	−3	6
			2						1		−2					
									1	−1			1			
									1		2	−4		−4	−4	8
19		1														
29	1	2		−1		−1		1								
	1		−2	1		−1		3		−2		4		2		−4
36	1		−2	1		−1	1				1	−1		1	−1	
38	1	−2	−1	−1		−1	2	−1						2		−2
51		1														
	1		−1													
					1											
						1	1	−2								
	1								−1							
				1					−1	1	1	−1	1	−1	−1	
						1						1	1	−1	−1	
							1			−1		1		1	−1	
72		1						−1								
76	1			−1												
		1						−1								
		1	1			−1						−1				
		1	−1					−1							1	
			1													−1
108	1			1		1	−1				−1	2			2	−3
132			1	−1		1	−1							−1		1
140	1	1														
			1	−1		1		−1								
					1		−1			1				−1		
172	1	1	−1	1												
200		1														
				1												
								1								
														1		
																1
204								any								

Table 3: Staggered invariants of type $(2,1)$ up to range $\alpha = 4$ for ECA.

Rule	b_0	b_1	b_2	b_3	b_4	b_5	b_6	b_7	b_8	b_9	b_{10}	b_{11}	b_{12}	b_{13}	b_{14}	b_{15}	b_{16}
1	1	−4	2			−2	2	2	−2								
3	1	−3	1	−1	1												
		1	−2	−2	3	−1	2	2	−3			1	−1			−1	1
5	1	−3		1						−1		1					
15	1	−2															
		1		−1	−2	−2	4										
			1		−2	−1	2										
							1	−1									
			1					−1	−2	−2	3	2	−1		−1	−1	1
		1						−4		−3	4	2					
					1				−2	−1	2	1	−1		−1	−1	2
											1			−1			
19	1		−4	−6	8		2	2	−4			2	−2			−2	2
27	1	−3	3	−1	−1			1	−1								
29	1	−2															
		1	−1	−1			−1		2		−1		2		1		−2
38		1	−3	−1	3		1	2	−3						−2		2
51	1	−2															
		1		−1	−2	−2	4										
			1		−2	−1	2										
							1	−1									
			1					−1	−2	−2	3	2	−1		−1	−1	1
		1						−4		−3	4	2					
					1				−2	−1	2	1	−1		−1	−1	2
											1			−1			

Table 4: Staggered invariants of type $(2,2)$ up to range $\alpha = 4$ for ECA.

Rule	b_1	b_2	b_3	b_4	b_5	b_6	b_7	b_8	b_9	b_{10}	b_{11}	b_{12}	b_{13}	b_{14}	b_{15}	b_{16}
1		1				1	−1	−1	1							
2	1	1	−1	1												
5	1		−1						−1		1					
10	1		−1													
		1		1			−1	1								
15	1		−1													
		1														
					1											
						1	1	−2								
			1						−1							
				1					−1	1	1	−1	1	−1	−1	
						1						1		−1	−1	
								2		−1		2	1		−2	
19			1			1	−1				−1	1			1	−1
24	1	−1	−1			−1						−1	−1	1	1	
29	1	1	−1	1				−1		−1				1		
				1		1		−1								
34	1	1														
			1	−1		1		−1								
					1		−1			1				−1		
38	1	1	−1	1		−1		1								
42	1	1														
	1	−1		−2												
			1	−1		1										
					1		−1			1				−1		
						1		−1				1				−1
							1	−1						1		−1
46	1	1	−1	1		−1		1								
51	1															
		1			1	−1	−1									
			1	−2												
				2		1	−1									
					−2	1	1		−1				2			
						1	−1		−1			2		2	2	−4
									1	−1			−1			
										1	2	−4	1	−4	−4	8
138	1		−1	1												
		1					−1	1								
				1											−1	1
170	any															

4. Elementary reversible cellular automata

ERCA are another example of CA of the form (1.2). In this case, $X = \{0,1\}^2$ and $x_i^t = (\sigma_i^t, \hat{\sigma}_i^t)$, where σ_i^t and $\hat{\sigma}_i^t$ take values in the set $\{0,1\}$. The time evolution rule of ERCA is written as

$$\sigma_l^{t+1} = \hat{\sigma}_l^t \oplus f(\sigma_{l-1}^t, \sigma_l^t, \sigma_{l+1}^t) \tag{4.1}$$
$$\hat{\sigma}_l^{t+1} = \sigma_l^t \tag{4.2}$$

where $f : \{0,1\}^3 \to \{0,1\}$ is an arbitrary function and $\oplus$ denotes the exclusive OR operation (i.e., $1 \oplus 0 = 0 \oplus 0 = 1, \quad 1 \oplus 1 = 0 \oplus 0 = 0$). Each rule is named by the rule number given by equation (3.1) where f replaces g, followed by an R. There are 256 rules for ERCA and again the reflection and boolean conjugation symmetries are used to classify them into 88 equivalence classes.

In this case, function F is generally developed as

$$\begin{aligned} &F(\sigma_0, \hat{\sigma}_0, \ldots, \sigma_\alpha, \hat{\sigma}_\alpha) \\ &\quad = b_0 + b_1\sigma_0 + b_2\hat{\sigma}_0 + b_3\sigma_0\hat{\sigma}_0 + b_4\sigma_0\sigma_1 + b_5\hat{\sigma}_0\sigma_1 + \cdots \\ &\quad = b_0 + \sum_{\substack{(a_0, \hat{a}_0, \ldots, a_\alpha, \hat{a}_\alpha) \in \{0,1\}^{2\alpha+2} \\ (a_0, \hat{a}_0) \neq (0,0)}} b_k \sigma_0^{a_0} \hat{\sigma}_0^{\hat{a}_0} \ldots \sigma_\alpha^{a_\alpha} \hat{\sigma}_\alpha^{\hat{a}_\alpha}, \end{aligned} \tag{4.3}$$

with the use of $3 \cdot 4^\alpha + 1$ parameters $\{b_k\}$, and k is the integer given by

$$k = a_0 + 2\hat{a}_0 + 3\sum_{i=1}^{\alpha}(a_i + 2\hat{a}_i)4^{i-1}. \tag{4.4}$$

As in the case of ECA, b_0 is not necessary if $\tau = 0$ or $\lambda \neq 1$.

The equations have been solved for $\{b_k\}$ in cases $(\tau, \lambda) = (1,1)$, $(1,2)$, $(2,1)$, and $(2,2)$, with range $\alpha \leq 2$ for each rule. The number of invariants obtained are shown in Table 5. The numbers of localized invariants of $\tau = 1$ are also shown for reference.

A remarkable feature seen in Table 5 is that every rule that has an additive conserved quantity also possesses staggered invariants of type $(1,2)$ and/or $(2,2)$. Moreover, there are some rules that have staggered invariants but do not have an additive conserved quantity. These facts are in contrast to the case of ECA. On the other hand, ERCA and ECA have in common the fact that most of the staggered invariants are induced by localized periodic functions.

Some staggered invariants are related with symmetries of the rules. Rules 90R, 95R, and 165R are the peripheral rules where the rule function $f(x,y,z)$ actually does not depend on y. Then the space-time pattern of $\{\sigma_l^t\}$ is separated into two independent regions like a checkerboard. Therefore, if such a rule has an additive conserved quantity, it is decomposed into two conserved quantities each defined on a component of the checkerboard, which are nothing but staggered invariants of type $(2,2)$.

Table 5: Number of staggered invariants for the range $\alpha = 2$ for ERCA. The numbers in parentheses in the column of type $(1,1)$ are the numbers of independent localized periodic functions of period 1.

Rule	Type (τ,λ)				Rule	Type (τ,λ)			
	$(1,1)$	$(1,2)$	$(2,1)$	$(2,2)$		$(1,1)$	$(1,2)$	$(2,1)$	$(2,2)$
0R	26(26)	26	22	22	**59R**	2(2)	2		
1R	16(15)	15	11	12	**60R**				
2R	11(11)	11	7	7	**61R**				
3R	8(8)	8	4	4	**62R**				
4R	13(13)	13	9	9	**63R**				
5R	7(7)	7	5	5	**73R**	2(1)	1		
6R	5(5)	5	2	2	**75R**				
7R	3(3)	3	1	1	**77R**	3(0)			1
9R	4(4)	4	1	1	**79R**				
10R	3(3)	3	2	2	**90R**	4(0)			4
11R	1(1)	1			**91R**	3(0)			2
12R	4(4)	4			**94R**	1(0)			1
13R					**95R**	2(0)			2
14R					**105R**				
15R					**107R**				
18R	6(5)	5	1	2	**109R**				
19R	9(9)	9	3	3	**111R**				
22R	3(2)	2			**123R**	2(0)			1
23R	4(4)	5	1		**126R**	4(2)	2	2	3
24R	2(2)	2		1	**127R**	4(2)	2	2	3
25R					**129R**	7(6)	6	3	3
26R	1(0)			1	**131R**	2(2)	2		
27R	2(2)	2			**133R**		1	1	
28R					**135R**				
29R					**139R**	1(1)	1		
30R					**141R**				
31R					**143R**				
33R	4(4)	5	1		**147R**	3(3)	3		
35R	4(4)	4			**151R**		1		
36R	7(6)	6	3	3	**153R**				
37R	3(2)	3	1	1	**155R**				
38R	2(2)	2			**157R**				
39R	2(2)	2			**159R**				
41R		1			**165R**	2(0)	2	2	2
43R					**167R**		1	1	
45R					**175R**		1	1	
46R	2(2)	2			**179R**	7(6)	6		1
47R					**183R**		2	1	
50R	8(6)	6			**187R**				
51R	16(16)	16			**189R**	1(1)	2	1	1
54R	3(2)	2			**191R**	1(1)	2	1	1
55R	5(4)	4			**219R**	4(2)	2	2	3
57R					**223R**	3(2)	2	2	2
58R					**255R**	12(12)	12	12	12

Table 6: Propagative staggered invariants of type $(1,2)$ up to $\alpha = 1$ for ERCA.

Rule	b_1	b_2	b_3	b_4	b_5	b_6	b_7	b_8	b_9	b_{10}	b_{11}	b_{12}
33R					1		1					
37R					1		1					
41R			1		−1		−1					
133R					1		1					
151R				2	1	−2	1	2	−2	−2	−2	2
165R	1	−1			2							
					1		1					
167R	1	−1			1		−1					
175R	1	−1			1		−1					
183R	1	−1			1		−1					
				2	1	−2	1	2	−2	−2	−2	2
189R	1	−1			1		−1					
191R	1	−1			1		−1					

Table 7: Staggered invariants of type $(2,1)$ up to $\alpha = 1$ for ERCA.

Rule	b_0	b_1	b_2	b_3	b_4	b_5	b_6	b_7	b_8	b_9	b_{10}	b_{11}	b_{12}
0R		1	−1										
						1		−1					
					1				−1				
							1			−1			
											1	−1	
1R						1		−1					
							1			−1			
											1	−1	
2R		1	−1			1		−1					
							1			−1			
3R							1			−1			
4R						1		−1					
					1		−1		−1	1	−1	1	
5R						1		−1					
10R		1	−1			1		−1					
33R						1		−1					
36R						1		−1					
					1		−1		−1	1	−1	1	
37R						1		−1					
126R				2		−1		−1					
127R				2		−1		−1					
129R						1		−1					
							1			−1	−1	1	
133R						1		−1					
165R	1	−2	−2			2		2					
						1		−1					
167R	1	−2	−2			2		2					
175R	1	−2	−2			2		2					
183R	1	−2	−2			2		2					
189R	1	−2	−2			2		2					
191R	1	−2	−2			2		2					
219R	1	−2	−2	2		1		1					
223R	1	−2	−2	2		1		1					
255R	1	−2	−2	4									
		1	−1		−1				1				
				2		−1		−1					

Table 8: Staggered invariants of type $(2,2)$ up to $\alpha = 1$ for ERCA.

Rule	b_1	b_2	b_3	b_4	b_5	b_6	b_7	b_8	b_9	b_{10}	b_{11}	b_{12}
0R	1	−1										
					1		−1					
				1				−1				
						1			−1			
										1	−1	
1R					1		−1					
						1			−1			
										1	−1	
2R	1	−1			1		−1					
						1			−1			
3R						1			−1			
4R					1		−1					
				1		−1		−1	1	−1	1	
5R					1		−1					
10R	1	−1			1		−1					
18R	1	−1			1		−1					
24R	1	−1			1		−1					
26R	1	−1			1		−1					
36R				1		−1		−1	1	−1	1	
90R	1	−1			1		−1					
					1		1					
91R					1		1					
94R					1		1					
95R					1		1					
123R					1		1					
126R					1		1					
127R					1		1					
129R					1	−1	−1		1	1	−1	
189R	1	1	−2		−1		−1					
191R	1	1	−2		−1		−1					
219R					1		1					
223R					1		1					
255R	1	1	−2									
					1		1					
				1				−1				

Another example is related to boolean complement symmetry [4]. For a function $f(x, y, z)$, we can write

$$\overline{f}(x, y, z) = 1 - f(x, y, z). \tag{4.5}$$

Then, the rule specified by $\overline{f}$ (rule $\overline{f}$R) is called the *complement* of the rule specified by f (rule fR). Note that this is different from the boolean conjugation operation or the exchange of the roles of 0 and 1. The latter is executed by

$$h(x, y, z) = f(1 - x, 1 - y, 1 - z). \tag{4.6}$$

Let $\{\sigma_i^t\}$ be an orbit in rule fR. If $\{\nu_l^t\}$ is defined by

$$\nu_l^t = \begin{cases} \sigma_l^t & \text{for} \quad t = 4n \text{ or } 4n+1 \\ 1 - \sigma_l^t & \text{for} \quad t = 4n+2 \text{ or } 4n+3, \end{cases} \tag{4.7}$$

and n is an integer, $\{\nu_l^t\}$ satisfies the following relation

$$\nu_l^t = \begin{cases} \overline{f}(\nu_{l-1}^t, \nu_l^t, \nu_{l-1}^t) \oplus \nu_l^{t-1} & \text{for} \quad t = 4n \text{ or } 4n+1 \\ \overline{h}(\nu_{l-1}^t, \nu_l^t, \nu_{l-1}^t) \oplus \nu_l^{t-1} & \text{for} \quad t = 4n+2 \text{ or } 4n+3. \end{cases} \tag{4.8}$$

This relation means that if rules $\overline{f}$R and $\overline{h}$R have an additive conserved quantity in common, rule fR has a staggered invariant of $\tau = 4$ or 2. If the density F is symmetric in transformation $(\sigma_l, \hat{\sigma}_l) \leftrightarrow (1 - \sigma_l, 1 - \hat{\sigma}_l)$, period τ becomes 2. This is the case for rules 165R, 167R, 175R, 183R, 189R, and 191R, where $f(x, y, z) = 1$ if $x \oplus z = 0$. Because their complements have the additive conserved quantity

$$\Phi(\mathbf{x}^t) = \sum_l \left[(\sigma_l^t - \hat{\sigma}_{l+1}^t)^2 + (\hat{\sigma}_l^t - \sigma_{l+1}^t)^2 \right] \tag{4.9}$$

in common, $(-1)^t \Phi$ must be a staggered invariant, or a sum of a staggered invariant and an additive conserved quantity. However, because these rules do not have an additive conserved quantity of this range, $(-1)^t \Phi$ is a staggered invariant.

In additon to those previously mentioned, there are some staggered invariants that commonly appear in a number of rules:

(a) The rules where $f(x, y, z) = 0$ if $x \oplus z = 0$ have the staggered invariant of type $(2, 2)$

$$\Psi(\mathbf{x}^t) = (-1)^t \sum_l (-1)^l \left[(\hat{\sigma}_l^t - \sigma_{l+1}^t)^2 - (\sigma_l^t - \hat{\sigma}_{l+1}^t)^2 \right] \tag{4.10}$$

besides the additive conserved quantity (4.9).

(b) The rules where $f(x, y, z) = 1$ if $x \oplus z = 1$ have the staggered invariant

$$\Psi(\mathbf{x}^t) = (-1)^t \sum_l (-1)^l \left[(\sigma_l^t - \hat{\sigma}_{l+1}^t)^2 + (\hat{\sigma}_l^t - \sigma_{l+1}^t)^2 \right] \tag{4.11}$$

as well as the additive conserved quantity

$$\Phi(\mathbf{x}^t) = \sum_l \left[(\hat{\sigma}_l^t - \sigma_{l+1}^t)^2 - (\sigma_l^t - \hat{\sigma}_{l+1}^t)^2 \right]. \tag{4.12}$$

These may also have some relation to symmetries.

5. Discussion

In this paper a necessary and sufficient condition has been derived so that a CA has staggered invariants and it has shown that the condition is written in the form of the equation of continuity. Moreover, the condition has been applied to ECA and ERCA to obtain the staggered invariants in the case that α, τ, and λ are relatively small. The staggered invariants in ECA is related to space-time patterns of the class-2 rules, while the case of ERCA contains some nontrivial examples.

Although I have solved the conservation condition for ECA and ERCA only in the case that $\tau \leq 2$ and $\lambda \leq 2$, it turns out that staggered invariants with larger τ or λ also exist. As stated in section 2, a localized periodic function of period τ (if it exists) becomes a density function for a staggered invariant of type (τ, λ) with an arbitrary λ. Thus there is no upper bound of λ. Concerning τ, there is at least a case with $\tau = 4$. It is found in rule 255R, where the rule function is $f(x, y, z) = 1$ for any (x, y, z) and each site changes its value with period four independently of other sites. Except for the case of a localized periodic function, there may be an upper bound for τ and λ, though I do not know how to determine it.

Let us consider the possibility of the extension of the conservation condition. The extension to rules with a wider interaction range is straightforward. The case of additive conserved quantities was already discussed in [2]. The conservation condition of staggered invariants can be extended in the same manner. The extension to higher dimensions is another possibility. I expect that the condition then can also be written in the form of the equation of continuity, where current J must be a vector.

In mechanical systems, as mentioned in the introduction, conserved quantities are connected with the symmetries of the system considered via Noether's theorem. Thus, one may find such a relation also in the case of CA, though the conditions obtained in this paper do not clearly suggest it. If one can unveil that possible connection hidden in the present condition, it will provide us with a unified view for the invariants of dynamical systems.

ERCA preserve the phase space volume. Hence, if a rule has an additive conserved quantity, one can develop standard statistical mechanics there. By comparison of simulation results with statistical mechanics predictions,

one can discuss the relation between microscopic dynamics and ergodicity. I have simulated equilibrium and nonequilibrium thermodynamic properties of the seven rules 26R, 77R, 90R, 91R, 94R, 95R, and 123R, which have additive conserved quantities of $\alpha = 1$ but do not have a localized periodic function in any range α[13, 14, 15]. Table 2 shows that *all* these rules have staggered invariants of type (2,2). It is interesting to investigate how these staggered invariants affect the thermodynamic behavior of the rules. Under the boundary condition where heat baths are attached at both the ends, no significant effects have been observed [16]. The effect should be subtle, if any. Possible roles on the behavior of other rules are a future problem.

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