Ultradiscrete two-variable Oregonator

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Abstract

Ultradiscretization is a limiting procedure transforming a given differential/difference equation into a ultradiscrete equation. Ultradiscrete equations are expressed by addition, subtraction and/or max. The procedure is expected to preserve the essential properties of the original equations. As a method of ultradiscretization, there is "tropical discretization" proposed by M. Murata. In this paper, we shall modify it, and derive a ultradiscrete equation from the continuous model of the BZ reaction. The derived equation generates a cellular automaton by restricting the values of the parameters, which is equivalent to one of those introduced by D. Takahashi, A. Shida, and M. Usami. By setting appropriate initial values, we can obtain the patterns of BZ reaction.

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Key words: discretization, ultradiscrete equation, BZ reaction, cellular automaton.

1 Introduction

Ultradiscretization is a limiting procedure transforming a given differential/difference equation into a ultradiscrete equation. Ultradiscrete equations are based on the max-plus algebra, which defines the summation by max and the product by +, and often expressed in simple forms. It is expected that this procedure preserves the essential properties of the original equations. In the reaction-diffusion system, both continuous models using partial differential equations and mathematical models using cellular automata have been studied. However, the direct correspondence between them is not clear. Indeed, it was difficult to obtain max-plus equations expressing the BZ reaction directly from the system of partial differential equations. For example, in their paper [3], D. Takahashi, A. Shida, and M. Usami created max-plus equations for the BZ reaction by comparing the nature.
As a method of ultradiscretization, there is “tropical discretization” proposed by M. Murata [1, 2]. In this paper, we shall modify it, and derive a ultradiscrete equation from the continuous model of the BZ reaction. Ultradiscretization of two-dimensional space diffusion terms will be the mean of values of neighbouring four points and center. In Murata’s method, the value of center is not used. Another difference is which terms are shifted in time. The derived equation generates a cellular automaton by restricting the values of the parameters, which is equivalent to one of those introduced in the paper [3]. By setting appropriate initial values, we obtain the patterns of BZ reaction, ring, target and spiral, which are mentioned in the book [4].

2 The two-variable Oregonator

The two-variable Oregonator in two-dimensional space is given by

\[
\begin{align*}
\frac{\partial u}{\partial t} &= D_u \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + a \left\{ u(1 - u) - \frac{fv(u - q)}{u + q} \right\}, \\
\frac{\partial v}{\partial t} &= D_v \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + u - v,
\end{align*}
\]

(2.1)

where \( u = u(t, x, y) \) is the activity factor and \( v = v(t, x, y) \) is the inhibitory factor. The constants \( D_u \) and \( D_v \) are the diffusion coefficients of \( u \) and \( v \), respectively. We consider \( (x, y) \in \mathbb{R}^2, t \geq 0 \) and the constants \( a, f, q \) satisfy \( a \sim 0.25 \times 10^2, 1 < f < 2, q \sim 8 \times 10^{-4} \). This system is known as a model to explain the pattern dynamics of the BZ reaction. The solutions of this system represent spatial patterns. Changing initial values and the values of parameters, we can observe various patterns.

2.1 Discretization

In this section, we discretize the eq. (2.1) by a method similar to Murata’s [1]. First we consider a discretization of the following system of partial differential equations:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= D_u \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \quad (D_u > 0), \\
\frac{\partial v}{\partial t} &= D_v \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \quad (D_v > 0).
\end{align*}
\]

(2.2)

The following system of difference equations is that.

\[
\begin{align*}
u_{n+1}^{i,k} &= \frac{1}{5} (u_{n}^{i,k} + u_{n}^{i-\alpha,k} + u_{n}^{i+\alpha,k} + u_{n}^{i,k-\alpha} + u_{n}^{i,k+\alpha}) = m_\alpha (u_{n}^{i,k}), \\
v_{n+1}^{j,k} &= \frac{1}{5} (v_{n}^{j,k} + v_{n}^{j-\beta,k} + v_{n}^{j+\beta,k} + v_{n}^{j,k-\beta} + v_{n}^{j,k+\beta}) = m_\beta (v_{n}^{j,k}).
\end{align*}
\]

(2.3)
Indeed, if we put $u_{n}^{j,k} = u(t, x, y)$ with $t = n\Delta t$, $x = j\Delta x$, $y = k\Delta y$ ($\Delta x = \Delta y$), we find

\[
\begin{align*}
    u_{n+1}^{j,k} &= u(t + \Delta t, x, y), \\
    u_{n}^{j\pm\alpha,k} &= u(t, x \pm \alpha\Delta x, y), \\
    u_{n}^{j,k\pm\alpha} &= u(t, x, y \pm \alpha\Delta y).
\end{align*}
\]

By the taylor expansions at $(t, x, y)$, we get

\[
\begin{align*}
u(t, x, y) &= u, \\
u(t + \Delta t, x, y) &= u + u_t\Delta t + \frac{1}{2}u_{tt}\Delta t^2 + \cdots, \\
u(t, x \pm \alpha\Delta x, y) &= u \pm u_x\alpha\Delta x + \frac{1}{2}u_{xx}\alpha^2\Delta x^2 + \cdots, \\
u(t, x, y \pm \alpha\Delta y) &= u \pm u_y\alpha\Delta y + \frac{1}{2}u_{yy}\alpha^2\Delta y^2 + \cdots.
\end{align*}
\]

Substituting them into the eq.(2.3), we get

\[
\begin{align*}
u + u_t\Delta t + \frac{1}{2}u_{tt}\Delta t^2 + \cdots &= \frac{1}{5}\left\{ u + \left( u + u_x\alpha\Delta x + \frac{1}{2}u_{xx}\alpha^2\Delta x^2 + \cdots \right) \\
&\quad + \left( u - u_x\alpha\Delta x + \frac{1}{2}u_{xx}\alpha^2\Delta x^2 - \cdots \right) \\
&\quad + \left( u + u_y\alpha\Delta y + \frac{1}{2}u_{yy}\alpha^2\Delta y^2 + \cdots \right) \\
&\quad + \left( u - u_y\alpha\Delta y + \frac{1}{2}u_{yy}\alpha^2\Delta y^2 - \cdots \right) \right\},
\end{align*}
\]

and thus

\[
\begin{align*}
u_t + \cdots &= \frac{1}{5}u_{xx}\alpha^2\Delta x^2 + \frac{1}{5}u_{yy}\alpha^2\Delta y^2 + \cdots, \\
u_t + \cdots &= \frac{\alpha}{5\Delta t}u_{xx} + \frac{\alpha^2\Delta y^2}{5\Delta t}u_{yy} + \cdots, \\
\end{align*}
\]

(2.4)

where $D = \alpha^2\Delta x^2/5\Delta t = \alpha^2\Delta y^2/5\Delta t$. Taking the limit $\Delta t, \Delta x, \Delta y \to 0$ without change of $D$, we obtain the first equation of the system eq.(2.2). Thus, the eq.(2.3) can be regarded as a discretization of the eq.(2.2).

Furthermore, we consider a discretization of the following system of ordinary differential equations:

\[
\begin{align*}
\frac{du}{dt} &= a \left\{ u(1-u) - \frac{fv(u-q)}{u+q} \right\}, \\
\frac{dv}{dt} &= u - v.
\end{align*}
\]

(2.5)
We shall show that the following system of difference equations is the required
\[
\begin{aligned}
\begin{cases}
    u_{n+1} = \frac{\varepsilon^{-1}u_n + au_n + afqv_n}{\varepsilon^{-1} + au_n + \frac{afv_n}{u_n + q}}, \\
v_{n+1} = \frac{\varepsilon^{-1}v_n + u_n}{\varepsilon^{-1} + 1},
\end{cases}
\end{aligned}
\] (2.6)

where \( n \in \mathbb{Z}_{\geq 0}, \varepsilon > 0 \). The method we adopt here is the same as that in the papers [1, 2].

Putting \( u_n = u(t), v_n = v(t), t = \varepsilon n \), we find
\[
\begin{aligned}
\begin{cases}
    \frac{u(t + \varepsilon) - u(t)}{\varepsilon} = a \left\{ \frac{u(t)(1 - u(t)) - f(v(t)(u(t) - q))}{u(t) + q} \right\} + O(\varepsilon), \\
    \frac{v(t + \varepsilon) - v(t)}{\varepsilon} = u(t) - v(t) + O(\varepsilon).
\end{cases}
\end{aligned}
\] (2.7)

Taking the limit \( \varepsilon \to +0 \), we obtain the system of differential equations (2.5). Thus, the eq. (2.6) can be regarded as a discretization of the eq. (2.5). Using the eq. (2.3) and the eq. (2.6), we will find the system of difference equations,
\[
\begin{aligned}
\begin{cases}
    u_{j,k}^{n+1} = \frac{\varepsilon^{-1}m_\alpha(u_{j,k}^{n}) + am_\alpha(u_{j,k}^{n}) + \frac{afqv_{j,k}^{n}}{m_\alpha(u_{j,k}^{n}) + q}}{\varepsilon^{-1} + am_\alpha(u_{j,k}^{n}) + \frac{afv_{j,k}^{n}}{m_\alpha(u_{j,k}^{n}) + q}}, \\
v_{j,k}^{n+1} = \frac{\varepsilon^{-1}m_\beta(v_{j,k}^{n}) + m_\beta(u_{j,k}^{n})}{\varepsilon^{-1} + 1}.
\end{cases}
\end{aligned}
\] (2.8)

This can be rewritten as
\[
\begin{aligned}
\begin{cases}
    \frac{u_{j,k}^{n+1} - u_{j,k}^{n}}{\varepsilon} = m_\alpha(u_{j,k}^{n}) - u_{j,k}^{n} + a \left\{ m_\alpha(u_{j,k}^{n})(1 - u_{j,k}^{n}) - \frac{fv_{j,k}^{n}(u_{j,k}^{n} - q)}{m_\alpha(u_{j,k}^{n}) + q} \right\} + O(\varepsilon), \\
    \frac{v_{j,k}^{n+1} - v_{j,k}^{n}}{\varepsilon} = m_\beta(v_{j,k}^{n}) - v_{j,k}^{n} + m_\beta(u_{j,k}^{n}) - v_{j,k}^{n} + O(\varepsilon),
\end{cases}
\end{aligned}
\] (2.9)

and thus can be regarded as a discretization of the eq. (2.1).

2.2 Ultradiscretization

In this section, we shall ultradiscretize the eq. (2.8) and investigate the solutions.

Let
\[
\begin{aligned}
u_{j,k}^{n} = \exp(U_{j,k}^{n}/\lambda), & \quad v_{j,k}^{n} = \exp(V_{j,k}^{n}/\lambda), \quad \varepsilon = \exp(E/\lambda), \\
a = \exp(A/\lambda), & \quad f = \exp(F/\lambda), \quad q = \exp(Q/\lambda),
\end{aligned}
\] (2.10)
and take the limit $\lambda \to +0$. Operations such as
\[
\lim_{\lambda \to +0} \lambda \log \left( e^{A/\lambda} + e^{B/\lambda} \right) = \max(A, B),
\]
\[
\lim_{\lambda \to +0} \lambda \log \left( e^{A/\lambda} \cdot e^{B/\lambda} \right) = A + B,
\]
\[
\lim_{\lambda \to +0} \lambda \log \left( e^{A/\lambda} / e^{B/\lambda} \right) = A - B,
\]
perform here. Therefore, the eq.(2.8) is transformed into
\[
U_{n+1}^{j,k} = \max\{M_\alpha(U_n^{j,k}) - E, A + M_\alpha(U_n^{j,k}), A + F + Q + V_n^{j,k} - \max(M_\alpha(U_n^{j,k}), Q)\}
\]
\[
- \max\{-E, A + M_\alpha(U_n^{j,k}), A + F + V_n^{j,k} - \max(M_\alpha(U_n^{j,k}), Q)\},
\]
\[
V_{n+1}^{j,k} = \max\{M_\beta(V_n^{j,k}) - E, M_\beta(U_n^{j,k})\} - \max\{-E, 0\},
\]
(2.11)
where
\[
M_\alpha(U_n^{j,k}) = \max(U_n^{j,k}, U_n^{j-\alpha,k}, U_n^{j+\alpha,k}, U_n^{j,k-\alpha}, U_n^{j,k+\alpha}),
\]
\[
M_\beta(V_n^{j,k}) = \max(V_n^{j,k}, V_n^{j-\beta,k}, V_n^{j+\beta,k}, V_n^{j,k-\beta}, V_n^{j,k+\beta}),
\]
which is an ultradiscretization of the eq.(2.3).

Taking the limit $E \to +\infty$, we get
\[
U_{n+1}^{j,k} = \max\{M_\alpha(U_n^{j,k}), F + Q + V_n^{j,k} - \max(M_\alpha(U_n^{j,k}), Q)\}
\]
\[
- \max\{M_\alpha(U_n^{j,k}), F + V_n^{j,k} - \max(M_\alpha(U_n^{j,k}), Q)\},
\]
(2.12)
and the following single ultradiscrete equation:
\[
U_{n+1}^{j,k} = \max\{M_\alpha(U_n^{j,k}), F + Q + M_\beta(U_{n-1}^{j,k}) - \max(M_\alpha(U_n^{j,k}), Q)\}
\]
\[
- \max\{M_\alpha(U_n^{j,k}), F + M_\beta(U_{n-1}^{j,k}) - \max(M_\alpha(U_n^{j,k}), Q)\}. 
\]
(2.13)

3 Cellular automaton

Considering the values of $f$ and $q$ in the eq.(2.1), we suppose $Q < 0 < F$ in the eq.(2.13). We take $Q = -1$, $F = 1$, and restrict initial values to $U_0^{j,k}, U_1^{j,k} \in \{-1, 0\}$ to generate a cellular automaton. Under this condition, the values of $U_n^{j,k}$ are restricted to $\{-1, 0\}$. To shift the values to $\{0, 1\}$, Let
\[
W_n^{j,k} = U_n^{j,k} - Q,
\]
(3.1)
and substitute it into the eq.(2.13). We get
\[
W_{n+1}^{j,k} = \max\{M_\alpha(W_n^{j,k}), F + M_\beta(W_{n-1}^{j,k}) - M_\alpha(W_n^{j,k})\}
\]
\[
- \max\{M_\alpha(W_n^{j,k}) + Q, F + M_\beta(W_{n-1}^{j,k}) - M_\alpha(W_n^{j,k})\}. 
\]
(3.2)
Since we find
\[ M_\alpha(W_{j,k}^n) \in \{0, 1\}, \]
\[ F + M_\beta(W_{j,k}^{n-1}) - M_\alpha(W_{j,k}^n) \in \{0, 1, 2\}, \]
\[ M_\alpha(W_{j,k}^n) + Q \in \{-1, 0\}, \]
it follows that
\[ F + M_\beta(W_{j,k}^{n-1}) - M_\alpha(W_{j,k}^n) \geq M_\alpha(W_{j,k}^n) + Q. \]

Therefore, we obtain the following simple equation:
\[ W_{j,k}^{n+1} = \max\{2M_\alpha(W_{j,k}^n) - M_\beta(W_{j,k}^{n-1}) - F, 0\}. \] (3.3)

The rule of time evolution is in the Table 3.1:

| \( M_\alpha(W_{j,k}^n), M_\beta(W_{j,k}^{n-1}) \) | 0, 0 | 0, 1 | 1, 0 | 1, 1 |
|---------------------------------------------|-----|-----|-----|-----|
| \( W_{j,k}^{n+1} \)                        | 0   | 0   | 1   | 0   |

Table 3.1: \( W_{j,k}^{n+1} \)

We shall compare it with one of Takahashi, Shida and Usami’s max-plus equations [3]:
\[ Y_{j,k}^{n+1} = \max(Y_{j,k}^n, Y_{j,k-1}^n, Y_{j,k+1}^n, Y_{j-1,k}^n, Y_{j+1,k}^n) - Y_{j,k}^{n-1}. \] (3.4)

We recall that this equation was not associated with the differential equation directly. Using our terminology, we obtain the following form:
\[ Y_{j,k}^{n+1} = \max(M_1(Y_{j,k}^n) - Y_{j,k}^{n-1}, 0) . \] (3.5)

The rule of time evolution is in the Table 3.2:

| \( M_1(Y_{j,k}^n), Y_{j,k}^{n-1} \) | 0, 0 | 0, 1 | 1, 0 | 1, 1 |
|----------------------------------|-----|-----|-----|-----|
| \( Y_{j,k}^{n+1} \)             | 0   | 0   | 1   | 0   |

Table 3.2: \( Y_{j,k}^{n+1} \)

In the case of \((\alpha, \beta) = (1, 0)\) the rules are the same. Therefore, we have found a connection between the cellular automaton and the two-variable Oreg-onator by toropical discretization. For reader’s convenience, we shall introduce examples of simulation, because there is no example for this cellular automaton in the paper [3]. The following are introduced in the text-book [4].

The Figure 3.1 shows a ‘single ring’ pattern. From the center, a square-shaped wave with value 1 spreads outwards.
Figure 3.1: Single ring pattern.

The Figure 3.2 shows a process to form a stable ‘target’ pattern. At the center, the value changes periodically as 1,1,0,0 and square-shaped waves appear and spread outwards repeatedly with period 4.

Figure 3.2: Target pattern.

The Figure 3.3 shows a process to form a stable ‘spiral’ pattern. By a half-line cut from an infinite line of value 1, a spiral appears from its end point. After infinite time, the spiral spreads through the whole space region and it rotates by 90 degrees per unit time.

Figure 3.3: Spiral pattern.
The behavior of these solutions is similar to that of BZ reaction patterns.

4 Solutions without diffusion effect

The eq.(3.3) with $(\alpha, \beta) = (0, 0)$ is equivalent to

$$
Z_{n+2} = \max\{2Z_{n+1} - Z_n - F, 0\} \quad (Z_n \geq 0),
$$

(4.1)
at each point, which can be regarded as the equation without diffusion effect.

We observe the behavior of the solutions.

In the case of $2Z_{n+1} - Z_n - F \leq 0$, it follows that

$$Z_{n+2} = 0$$
$$Z_{n+3} = \max(2 \cdot 0 - Z_{n+1} - F, 0) = 0$$
$$Z_{n+4} = \max(2 \cdot 0 - 0 - F, 0) = 0$$

$\vdots$

Therefore, once the solution gets 0, it keeps 0 all the time.

In the case of $2Z_{n+1} - Z_n - F > 0$, we get

$$Z_{n+2} = 2Z_{n+1} - Z_n - F.$$

(4.2)
Let the initial value be \((Z_0, Z_1) = (a, b) \ (a, b \geq 0)\). The general solution is
\[
Z_n = -\frac{1}{2}Fn^2 + \left(\frac{1}{2}F - a + b\right)n + a. \tag{4.3}
\]

Taking the limit \(n \to \infty\), we get
\[
\lim_{n \to \infty} Z_n = -\infty.
\]

However, this result contradicts that \(Z_n\) are not negative. Therefore, we obtain
\[
\lim_{n \to \infty} Z_n = 0.
\]

We consider \((Z_0, Z_1) = (0, 3)\) as an example, we get
\[
0 \to 3 \to 5 \to 6 \to 6 \to 5 \to 3 \to 0 \to 0 \to \cdots.
\]

Firstly it reaches a certain value, secondly monotonically decreases therefrom and finally converges to 0.

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