Mechanism Generating Spatial Patterns in Reaction-Diffusion Systems

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In 1952, A. M. Turing proposed the notion of “diffusion-driven instability” in his attempt of modeling biological pattern formation. Following his ingenious idea, many reaction-diffusion systems have been proposed later on. On the other hand, Turing patterns can be explained by some cellular automata. Cellular automata are theoretical models which consist of a regular grid of cells, and they exhibit the complex behavior from quite simple rules. In this paper, we describe the mathematical properties of reaction-diffusion systems modeling pattern formation, in particular, Turing patterns. Moreover, we explain ideas which connect differential equations with cellular automata.

KEYWORDS: pattern formation, activator-inhibitor system, cellular automata

1. Introduction

1.1 Pattern formation

In biology, the development of patterns and forms is caused by chemical reactions inside cells and communications among cells. It is one of the most interesting subjects to understand the mechanism of morphogenesis, which is the part of embryology. A. M. Turing [15] wanted to understand how it is possible that a symmetric embryo evolves an asymmetric form, and proposed the idea of diffusion driven instability in his seminal paper in 1952. It is explained as follows. The reaction between two chemicals with different diffusion rates may cause the destabilization of a spatially homogeneous state, thus leading to the formation of nontrivial spatial structures. His idea was demonstrated by using a linear reaction-diffusion system, however, many other systems based on his idea have been proposed later on. Spatial patterns generated by that idea have been often called Turing patterns, and they have the following fundamental properties:

- They are the stationary spatial structures generated by reaction-diffusion systems.
- Small inhomogeneous perturbations to a stable steady state in kinetic system grow in the presence of diffusion.
- They have intrinsic wavelength determined by parameters of the reaction-diffusion process, which does not depend on boundary conditions, external forces.

These insights provide, for example, a possible mechanism for producing patterns in animal skin. Original observation of the dynamic properties of Turing patterns in nature was made by Kondo and Asai [8] in 1995. They explained the mechanism of the formation of horizontal stripes in the tropical fish Pomacanthus imperator (Figure 1.1) by using a reaction-diffusion system based on Turing’s idea. Since stripe patterns on Pomacanthus imperator are not fixed in their skin, they maintain the spaces between the lines by the continuous rearrangement of patterns. This phenomenon is predicted by numerical simulations. On the other hand, concerning stripe patterns on zebra, Turing instability is exhibited in the early stages of embryonic development—around 21–35 days of gestation. The visible stripes on zebra enlarge proportionally during its body growth. This is not a Turing patterning mechanism because it contradicts the third property of Turing patterns listed above.

In order to obtain Turing patterns under laboratory conditions, it is required that diffusion constants of the two species have a sufficiently large ratio. However, small molecules or ions all diffuse more or less at the same rate. Therefore, no clear experimental evidence of stationary Turing structures had been reported until the work of De Kepper and coworkers [1] in 1990. They used the chlorite-iodide-malonic acid starch (CIMA) reaction in an open unstirred gel reactor to visualize Turing’s pattern. Starch (S), which is used as a color indicator for the concentration of iodide (I\(^{-}\)) ion, forms a complex with iodide according to the scheme
The SI\textsuperscript{3} complex is considered to be practically immobile in the gel. On the other hand, chlorite (ClO\textsubscript{2}) is uncomplexed iodide. It can be easily seen that the diffusion of immobile molecules is substantially slower than that of chemicals which are not bound.

The CIMA reaction is described by a five-variable model involving the concentrations of I\textsuperscript{-}, ClO\textsubscript{2\textsuperscript{-}}, MA, ClO\textsubscript{2\textsuperscript{2}} and I\textsubscript{2}. Lengyel and Epstein [9] simplified the model to a two-variable model:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= D_1 \frac{\partial^2 u}{\partial x^2} - u - \frac{4 u v}{1 + u^2} + a, \\
\frac{\partial v}{\partial t} &= \delta \left[ D_2 \frac{\partial^2 v}{\partial x^2} + b \left( u - \frac{u v}{1 + u^2} \right) \right].
\end{align*}
\]

Here, \(D_1, D_2, \delta, a, b\) are positive constants. The unknown functions \(u(x, t)\) and \(v(x, t)\) represent the concentrations of iodide (I\textsuperscript{-}) and chlorite (ClO\textsubscript{2\textsuperscript{-}}) ions, respectively. \(\delta\) is a rescaling parameter which primarily depends upon the concentration of starch. The higher starch concentration means larger \(\delta\). Since the diffusion constant for \(v\) is \(\delta D_2\), it is much larger then the diffusion constant for \(u\) if the concentration of starch is sufficiently high.

As an example which generates a different kind of pattern, the Belousov–Zhabotinsky reaction (the BZ reaction) is famous as a spatio-temporal chemical oscillator. A typical recipe of the BZ reaction is the mixture of Ce\textsuperscript{4\textsuperscript{+}}, BrO\textsubscript{3\textsuperscript{2}}, \(\text{CH}_2(\text{COOH})_2\) and \(\text{H}_2\text{SO}_4\). In a thin unstirred layer of reaction solution, self-organized target patterns or spiral waves are developed. The Oregonator is known as a mathematical model which helps us to understand how the BZ reaction produces oscillations and waves (see e.g., [2]):

\[
\begin{align*}
\frac{dx}{dt} &= qy - xy + x(1 - x), \\
\frac{dy}{dt} &= -gy - xy + 2fz, \\
\frac{dz}{dt} &= x - z.
\end{align*}
\]

Here, \(\varepsilon, \delta, q, f\) are positive constants, and the functions \(x = x(t), y = y(t)\) and \(z = (t)\) represent the concentrations of bromous acid (HBrO\textsubscript{2}), bromine ion (Br\textsuperscript{-}), cerium ion (Ce\textsuperscript{4\textsuperscript{+}}), respectively.

In the Oregonator modeling of the BZ reaction, it is assumed that there are a huge number of molecules, and the number of molecules is approximated by the density. But, this idea cannot be applied to the case where the number of molecules is limited. Concerning Turing’s pattern, it is analyzed by reaction-diffusion equations on uniform media, where it is assumed that the size of each cell is extremely small. However, it is natural to consider discrete models to explain the mechanism of Turing patterns when we discuss it in a microscopic scale. Cellular automata have been known as discrete models for pattern formation. A cellular automaton consists of a regular grid of cells. For each cell, a set of cells called “neighborhood” is defined relative to the specified cell. If a fixed rule is given and an initial condition...
is selected by assigning a state for each cell, a new state of each cell is determined by the current state of the cell and the states of the cells in its neighborhood. Turing patterns and BZ reactions can be simulated by some kinds of cellular automata. If the both, a reaction-diffusion system and a cellular automaton, produce similar spatial patterns, then it is interesting to understand a common mechanism in both models.

In Section 2, we describe the mathematical properties of reaction-diffusion equations which lead to Turing patterns. In Section 3, we study the Lengyel–Epstein model to illustrate that the diffusion driven instability occur and some spatial patterns can emerge. In the last section, we consider the relation between reaction-diffusion systems and discrete models.

2. Turing’s Idea: Diffusion Driven Instability

The diffusion phenomenon is expressed by the following differential equation:

\[
\frac{\partial u}{\partial t} = D \Delta u, \quad x \in \Omega, \quad t > 0.
\]

Here, \( \Omega \subseteq \mathbb{R}^n \) is an open set in the \( n \)-dimensional Euclidean space \( \mathbb{R}^n \). The function \( u = u(x,t) \) represents the concentration or the density of particles or a species at position \( x \) and at time \( t \). The symbol \( \Delta \) is the Laplace operator in \( \mathbb{R}^n \), which is defined by

\[
\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \quad \text{if } n = 2.
\]

The constant \( D > 0 \) denotes the diffusion rate. The diffusion describes the spread of particles from regions of higher concentration to regions of lower concentration, and enhance spatial homogeneity. Therefore, it is impossible to get the nonhomogeneous spatial patterns by a diffusion process, only.

In 1952, A. M. Turing discovered that the reaction between two chemicals with different diffusion rates may cause the destabilization of the spatially homogeneous states, and lead to the formation of nontrivial spatial structures. This surprising idea is called the diffusion driven instability. In order to explain this phenomenon, let us consider the following two component system:

\[
\begin{aligned}
\frac{\partial u}{\partial t} &= D_1 \Delta u + f(u,v), \quad x \in \Omega, \quad t > 0, \\
\frac{\partial v}{\partial t} &= D_2 \Delta v + g(u,v), \quad x \in \Omega, \quad t > 0.
\end{aligned}
\tag{2.1}
\]

The first terms on the right-hand sides of (2.1) model diffusion, and \( D_1 > 0 \) and \( D_2 > 0 \) denote the diffusion coefficients of \( u \) and \( v \), respectively. The second terms on the right-hand sides of (2.1) describe the reaction between \( u \) and \( v \), which will be always nonlinear. The system (2.1) is called reaction-diffusion equations. The ordinary differential equations corresponding to (2.1) are called as the kinetic system and are of the form:

\[
\begin{aligned}
\frac{du}{dt} &= f(u,v), \quad t > 0, \\
\frac{dv}{dt} &= g(u,v), \quad t > 0.
\end{aligned}
\tag{2.2}
\]

The following conditions are necessary to generate spatial patterns by the diffusion driven instability:

1. \( u \) and \( v \) have different diffusion rates, for example, \( D_1 \ll D_2 \);
2. if \( (\tilde{u}, \tilde{v}) \) is a stable steady state of (2.2), then it is unstable as a stationary solution of (2.1).

The diffusion driven instability is sometimes called the Turing instability, and the spatial patterns caused by the Turing instability are called Turing’s pattern. In the following, we formulate this problem mathematically and we discuss necessary conditions for the Turing instability.

2.1 Linearized stability of steady states to ODE system

We consider the following initial-value problem:

\[
\begin{aligned}
\frac{du}{dt} &= f(u,v), \\
\frac{dv}{dt} &= g(u,v), \\
u(0) &= a, \quad v(0) = b.
\end{aligned}
\tag{2.3}
\]

Let \( (\tilde{u}, \tilde{v}) \) be a steady state of (2.3), which is defined by the equations \( f(\tilde{u}, \tilde{v}) = 0 \) and \( g(\tilde{u}, \tilde{v}) = 0 \). Therefore, an intersection of the curves \( f(u,v) = 0 \) and \( g(u,v) = 0 \) in the \( uv \)-plane corresponds to a steady state.
Definition 2.1. Let \((\bar{u}, \bar{v})\) be a steady state of (2.3). It is said to be stable if for any \(\varepsilon > 0\), there exists \(\delta > 0\) such that a solution \((u(t), v(t))\) of (2.3) with initial data \((a, b)\) satisfying \(|(a, b) - (\bar{u}, \bar{v})| < \delta\) satisfies \(|(u(t), v(t)) - (\bar{u}, \bar{v})| < \varepsilon\) for all \(t > 0\). The steady state \((\bar{u}, \bar{v})\) is said to be unstable if it is not stable.

Moreover, if \((\bar{u}, \bar{v})\) is stable and satisfies \((u(t), v(t)) \rightarrow (\bar{u}, \bar{v})\) as \(t \rightarrow +\infty\), then it is called asymptotically stable.

In order to check the stability of \((\bar{u}, \bar{v})\), we use the linearization of (2.3) at \((\bar{u}, \bar{v})\). Letting
\[
 \begin{align*}
 u(t) &= \bar{u} + \varepsilon \phi(t), \\
 v(t) &= \bar{v} + \varepsilon \psi(t),
\end{align*}
\] and substituting (2.4) into (2.3), we have
\[
\varepsilon \frac{d\phi}{dt} = f(\bar{u} + \varepsilon \phi, \bar{v} + \varepsilon \psi),
\]
\[
\varepsilon \frac{d\psi}{dt} = g(\bar{u} + \varepsilon \phi, \bar{v} + \varepsilon \psi).
\]

The Taylor expansion of \(f(\bar{u} + \varepsilon \phi, \bar{v} + \varepsilon \psi)\) at \((\bar{u}, \bar{v})\) is
\[
f(\bar{u} + \varepsilon \phi, \bar{v} + \varepsilon \psi) = f(\bar{u}, \bar{v}) + \frac{\partial f}{\partial u}(\bar{u}, \bar{v})\varepsilon \phi + \frac{\partial f}{\partial v}(\bar{u}, \bar{v})\varepsilon \psi
\]
\[
+ \frac{1}{2} \left[ \frac{\partial^2 f}{\partial u^2}(\bar{u}, \bar{v})\varepsilon^2 \phi^2 + \frac{\partial^2 f}{\partial u \partial v}(\bar{u}, \bar{v})\varepsilon \phi \varepsilon \psi + \frac{\partial^2 f}{\partial v^2}(\bar{u}, \bar{v})\varepsilon^2 \psi^2 \right] + \cdots
\]
\[
= \varepsilon \left[ \frac{\partial f}{\partial u}(\bar{u}, \bar{v})\phi + \frac{\partial f}{\partial v}(\bar{u}, \bar{v})\psi \right] + O(\varepsilon^2),
\]
where \(f(\bar{u}, \bar{v}) = 0\) because \((\bar{u}, \bar{v})\) is an equilibrium of (2.3). Similarly, \(g(\bar{u} + \varepsilon \phi, \bar{v} + \varepsilon \psi)\) is expanded as follows:
\[
g(\bar{u} + \varepsilon \phi, \bar{v} + \varepsilon \psi) = \varepsilon \left[ \frac{\partial g}{\partial u}(\bar{u}, \bar{v})\phi + \frac{\partial g}{\partial v}(\bar{u}, \bar{v})\psi \right] + O(\varepsilon^2).
\]

Therefore, the equations in (2.3) become
\[
\begin{align*}
 \frac{d\phi}{dt} &= \frac{\partial f}{\partial u}(\bar{u}, \bar{v})\phi + \frac{\partial f}{\partial v}(\bar{u}, \bar{v})\psi + O(\varepsilon), \\
 \frac{d\psi}{dt} &= \frac{\partial g}{\partial u}(\bar{u}, \bar{v})\phi + \frac{\partial g}{\partial v}(\bar{u}, \bar{v})\psi + O(\varepsilon).
\end{align*}
\]
(2.5)
(2.6)

Here, we assume that \(\varepsilon > 0\) is sufficiently small and both \(\phi(t)\) and \(\psi(t)\) are bounded, for example they satisfy \(\phi^2(t) + \psi^2(t) \leq 1\). Then, terms \(O(\varepsilon)\) on the right-hand sides of (2.5) and (2.6) can be neglected. Hence, the following linearized system gives a good approximation to (2.3) around \((\bar{u}, \bar{v})\):
\[
\begin{align*}
 \frac{d\phi}{dt} &= \frac{\partial f}{\partial u}(\bar{u}, \bar{v})\phi + \frac{\partial f}{\partial v}(\bar{u}, \bar{v})\psi, \\
 \frac{d\psi}{dt} &= \frac{\partial g}{\partial u}(\bar{u}, \bar{v})\phi + \frac{\partial g}{\partial v}(\bar{u}, \bar{v})\psi.
\end{align*}
\]
(2.7)

Let \(L\) be the Jacobian matrix on the right-hand side of (2.7), that is,
\[
\begin{pmatrix}
 \frac{d\phi}{dt} \\
 \frac{d\psi}{dt}
\end{pmatrix}
= \begin{pmatrix}
 \frac{\partial f}{\partial u}(\bar{u}, \bar{v}) & \frac{\partial f}{\partial v}(\bar{u}, \bar{v}) \\
 \frac{\partial g}{\partial u}(\bar{u}, \bar{v}) & \frac{\partial g}{\partial v}(\bar{u}, \bar{v})
\end{pmatrix}
\]
\[
\left(\begin{array}{c}
 \frac{d\phi}{dt} \\
 \frac{d\psi}{dt}
\end{array}\right)
= \begin{pmatrix}
 \frac{\partial f}{\partial u}(\bar{u}, \bar{v}) & \frac{\partial f}{\partial v}(\bar{u}, \bar{v}) \\
 \frac{\partial g}{\partial u}(\bar{u}, \bar{v}) & \frac{\partial g}{\partial v}(\bar{u}, \bar{v})
\end{pmatrix}
\]
\[
\left(\begin{array}{c}
 \phi \\
 \psi
\end{array}\right)
= L \left(\begin{array}{c}
 \phi \\
 \psi
\end{array}\right).
\]

In the following theorem, we explain how to use eigenvalues of \(L\) to analyze the stability of \((\bar{u}, \bar{v})\).

**Theorem 2.2.**

(i) If the real parts of both eigenvalues of \(L\) are negative, then \((\bar{u}, \bar{v})\) is asymptotically stable.

(ii) If \(L\) has an eigenvalue with positive real part, then \((\bar{u}, \bar{v})\) is unstable.

(iii) If \(L\) has purely imaginary eigenvalues, then the stability of \((\bar{u}, \bar{v})\) cannot be determined by the eigenvalues only.

For simplicity, we denote \(\frac{\partial f}{\partial u}(\bar{u}, \bar{v}), \frac{\partial f}{\partial v}(\bar{u}, \bar{v}), \frac{\partial g}{\partial u}(\bar{u}, \bar{v})\) and \(\frac{\partial g}{\partial v}(\bar{u}, \bar{v})\) by \(f_u, f_v, g_u\) and \(g_v\), respectively. The eigenvalues of \(L\) are solutions \(\lambda\) to the characteristic equation
\[
\det(L - \lambda I) = 0,
\]
where the left-hand side is the determinant of the matrix \(L - \lambda I\) and \(I\) is the identity matrix. Therefore, \(\lambda\) is a solution of
\[
\lambda^2 - (f_u + g_v)\lambda + (f_u g_v - f_v g_u) = 0.
\]
(2.8)
The both of two roots of (2.8) have negative real parts if and only if
\[ f_u + g_v < 0 \quad \text{and} \quad f_u g_v - f_v g_u > 0. \]

On the other hand, \( \mathcal{L} \) has an eigenvalue with positive real part if and only if it satisfies

\[ \text{either} \quad f_u + g_v > 0 \quad \text{or} \quad f_u g_v - f_v g_u < 0. \]

### 2.2 Turing instability

We consider the following initial-boundary value problem:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= D_1 \frac{\partial^2 u}{\partial x^2} + f(u, v), & 0 < x < L, t > 0, \\
\frac{\partial v}{\partial t} &= D_2 \frac{\partial^2 v}{\partial x^2} + g(u, v), & 0 < x < L, t > 0, \\
\frac{\partial u}{\partial x} &= \frac{\partial v}{\partial x} = 0, & x \in \{0, L\}, t > 0, \\
& u(x, 0) = u_0(x), \quad v(x, 0) = v_0(x), & 0 < x < L.
\end{align*}
\tag{2.9}
\]

Here, we focus on the problem on one-dimensional region \([0, L]\) for \( L > 0 \). The functions \( u = u(x, t) \) and \( v = v(x, t) \) represent the concentrations of particles at position \( x \) and at time \( t \). \( D_1 \) and \( D_2 \) are positive, which denote the diffusion coefficients. The Neumann boundary condition is imposed in (2.9), which means that \( u \) and \( v \) cannot go out from nor come into the region through boundaries. The ordinary differential equations corresponding to (2.9) are (2.3). Indeed, a solution of (2.9) with initial data \((u_0(x), v_0(x)) = (a, b)\) is also a solution of (2.3) thanks to the boundary condition in (2.9).

Assume \((\bar{u}, \bar{v})\) is an asymptotically stable steady state of (2.3). Hence, we impose the following conditions on the nonlinear terms at the point \((\bar{u}, \bar{v})\):

\[ f_u + g_v < 0 \quad \text{and} \quad f_u g_v - f_v g_u > 0. \tag{2.10} \]

Here, we use the same notations as in the previous subsection. For the Turing instability, the stable equilibrium \((\bar{u}, \bar{v})\) has to be destabilized in the presence of unequal diffusions. To illustrate this phenomenon, we use the linearization of (2.9) at \((\bar{u}, \bar{v})\) again and we see that \((\bar{u}, \bar{v})\) becomes unstable thanks to diffusions. Let

\[ u(x, t) = \bar{u} + \varepsilon z(x, t), \quad v(x, t) = \bar{v} + \varepsilon w(x, t). \]

Substituting these new variables into (2.9), after some calculations as shown in the previous subsection, we obtain the linearized system of (2.9) at \((\bar{u}, \bar{v})\):

\[
\begin{align*}
\frac{\partial z}{\partial t} &= D_1 \frac{\partial^2 z}{\partial x^2} + \frac{\partial f}{\partial u}(\bar{u}, \bar{v}) z + \frac{\partial f}{\partial v}(\bar{u}, \bar{v}) w, & 0 < x < L, t > 0, \\
\frac{\partial w}{\partial t} &= D_2 \frac{\partial^2 w}{\partial x^2} + \frac{\partial g}{\partial u}(\bar{u}, \bar{v}) z + \frac{\partial g}{\partial v}(\bar{u}, \bar{v}) w, & 0 < x < L, t > 0, \\
\frac{\partial z}{\partial x} &= \frac{\partial w}{\partial x} = 0, & x \in \{0, L\}, t > 0.
\end{align*}
\tag{2.11}
\]

It follows from the theory of Fourier series that solutions of (2.11) can be expressed as

\[ z(x, t) = \sum_{n=0}^{\infty} z_n(t) \cos \frac{\pi n}{L} x, \quad w(x, t) = \sum_{n=0}^{\infty} w_n(t) \cos \frac{\pi n}{L} x. \tag{2.12} \]

This idea, which was introduced by J. Fourier, says that the spatial distribution can be expressed in terms of the sum of trigonometric functions, and the coefficient of each spatial frequency develops in time independently around the steady state. Substituting (2.12) into (2.11) and comparing the coefficients of \( \cos \frac{\pi n}{L} x \) on both sides of the resulting system, we obtain, for \( n = 0, 1, 2, \ldots \), that

\[
\frac{d}{dt} \begin{pmatrix} z_n \\ w_n \end{pmatrix} = \begin{pmatrix} -D_1 \left( \frac{\pi n}{L} \right)^2 + f_u & f_v \\ g_u & -D_2 \left( \frac{\pi n}{L} \right)^2 + g_v \end{pmatrix} \begin{pmatrix} z_n \\ w_n \end{pmatrix}. \tag{2.13}
\]

Since the case of \( n = 0 \) corresponds to (2.3), \((\bar{u}, \bar{v})\) is stable for \( n = 0 \) because of the assumption. If we have, for all \( n \geq 1 \), that

\[ -D_1 \left( \frac{\pi n}{L} \right)^2 + f_u - D_2 \left( \frac{\pi n}{L} \right)^2 + g_v < 0 \tag{2.14} \]

and
\[
\left(-D_1 \left(\frac{\pi n}{L}\right)^2 + f_v\right) \left(-D_2 \left(\frac{\pi n}{L}\right)^2 + g_v\right) - f_v g_u > 0. \tag{2.15}
\]

then \(z_0(x, t), w_0(x, t) \to (0, 0)\) as \(t \to +\infty\) for all \(n \geq 1\). This implies that \((\bar{u}, \bar{v})\) is an asymptotically stable stationary solution of (2.9). Thus, the diffusion driven instability never occurs. Note that inequality (2.14) is always satisfied because \(D_1 > 0\) and \(D_2 > 0\). Therefore, in order that \((\bar{u}, \bar{v})\) is unstable, it is sufficient that there exists at least one \(n \geq 1\) such that

\[
\left(-D_1 \left(\frac{\pi n}{L}\right)^2 + f_v\right) \left(-D_2 \left(\frac{\pi n}{L}\right)^2 + g_v\right) - f_v g_u < 0.
\]

After some calculations, we obtain

\[
\left(\frac{\pi n}{L}\right)^4 D_1 D_2 < \left(\frac{\pi n}{L}\right)^2 (f_v D_2 + g_v D_1) - (f_u g_v - f_v g_u).
\tag{2.16}
\]

Since it is clear that the left-hand side of (2.16) is positive, the right-hand side of (2.16) should be positive as well. It follows from (2.10) that \(f_u g_v - f_v g_u > 0\). Therefore, the first term on the right-hand side of (2.16) has to be positive. Noting that \(f_u + g_v < 0\) is also satisfied by (2.10), we see that the quantity \(f_u D_2 + g_v D_1\) is positive if and only if one of the \(f_u\) and \(g_v\) is positive and the other negative. Now, let us consider the case \(f_u > 0\) and \(g_v < 0\). Then, \(D_1\) and \(D_2\) should satisfy

\[
D_2 > -\frac{g_v}{f_u} D_1
\tag{2.17}
\]

to get the both

\[
f_u + g_v < 0 \quad \text{and} \quad f_u D_2 + g_v D_1 > 0.
\]

This implies that (2.17) is a necessary condition for the diffusion driven instability. If we suppose \(f_u < 0\) and \(g_v > 0\), then \(f_u D_2 + g_v D_1\) is positive provided that \(D_1 > -(f_u/g_v)D_2\).

Next we seek a sufficient condition for the diffusion driven instability under the conditions \(f_u > 0\) and \(g_v < 0\). Let \((\pi n/L)^2 = \lambda\) for a fixed \(n \geq 1\). We see that inequality (2.16) becomes

\[
D_1 D_2 \lambda^2 - (D_2 f_u + D_1 g_v) \lambda + (f_u g_v - f_v g_u) < 0.
\tag{2.18}
\]

Put \(\xi = \lambda D_1\) and \(\eta = \lambda D_2\). Then, this inequality may be regarded as

\[
\xi \eta - (\eta f_u + \xi g_v) + (f_u g_v - f_v g_u) < 0.
\tag{2.19}
\]

Let \(\eta = \gamma \xi\). Then, the left-hand side of (2.19) is equal to

\[
\phi(\xi; \gamma) = \gamma^2 \xi^2 - (\gamma f_u + g_v) \xi + (f_u g_v - f_v g_u).
\]

The quadratic equation \(\phi(\xi; \gamma) = 0\) in \(\xi\) has positive roots if and only if

\[
g_v + \gamma f_u > 0 \quad \text{and} \quad (g_v + \gamma f_u)^2 - 4\gamma (f_u g_v - f_v g_u) \geq 0.
\tag{2.20}
\]

Note that (i) \((g_v + \gamma f_u)^2 - 4\gamma (f_u g_v - f_v g_u) < 0\) if \(\gamma = -g_v/f_u > 0\), and (ii) \((g_v + \gamma f_u)^2 - 4\gamma (f_u g_v - f_v g_u) \to +\infty\) as \(\gamma \to +\infty\). Moreover, we have

\[
(iii) \quad \frac{d}{d\gamma} \left(\frac{g_v + \gamma f_u}{4\gamma}\right) = \frac{(\gamma f_u + g_v)(\gamma f_u - g_v)}{4\gamma^2} > 0,
\]

provided that \(\gamma f_u + g_v > 0\). Combining (i)–(iii), we obtain that there exists a unique \(\gamma_c > -g_v/f_u > 0\) such that \(\phi(\xi; \gamma_c) = 0\) has a positive double zero, and \(\phi(\xi; \gamma) = 0\) has two positive zeros \(0 < \xi_1 < \xi_2\) if \(\gamma > \gamma_c\). In fact, \(\gamma_c\) is a root of

\[
f_v^2 \gamma + 2(2 f_u g_v - f_v g_u) \gamma + g_v^2 = 0.
\]

It is noted that \(\gamma_c > 1\) due to the first condition of (2.20). Consequently, we see that if \(\gamma > \gamma_c\) and \(\xi_1 < \xi < \xi_2\), then \(\phi(\xi; \gamma) < 0\). In other words, if

\[
\frac{D_2}{D_1} > \gamma_c \quad \text{and} \quad \frac{\xi_1 L^3}{(\pi n)^2} < D_1 < \frac{\xi_2 L^3}{(\pi n)^2},
\]

then (2.16) is satisfied and the stationary solution \((\bar{u}, \bar{v})\) is unstable.

### 2.3 Activator-inhibitor system

We consider the mechanism of the pattern formation in (2.9) when \(f_u > 0\) and \(g_v < 0\). From the assumption (2.10), we have \(f_u g_v - f_v g_u > 0\). Therefore, \(f_v\) and \(g_u\) should satisfy \(f_v g_u < 0\). This means that the signs of \(f_v\) and \(g_u\) should be opposite. Hence, there are only two possibilities:
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where, the head-activating substance represented by this system to simulate the regeneration and transplantation experiments on assumed that a change in cells or tissue takes place in the region where the activator concentration is high. They used concentration as in Figure 2.1 are in agreement with experiments. in which the released substances themselves influence further release. The results with localized pattern of the activator

3. Lengyel–Epstein Model

A. Gierer and H. Meinhardt [3] developed Turing’s idea, proposing several reaction-diffusion systems to model the biological pattern formation. The following is an example:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= D_u \frac{\partial^2 u}{\partial x^2} - u + \frac{u^2}{v} + \sigma, & 0 < x < 1, t > 0, \\
\frac{\partial v}{\partial t} &= D_v \frac{\partial^2 v}{\partial x^2} - v + u^2, & 0 < x < 1, t > 0,
\end{align*}
\]

where, \(D_u, \tau, D_v\) and \(\sigma\) are positive constants. This is an activator-inhibitor system in which \(u = u(x, t)\) and \(v = v(x, t)\) represent the concentrations of an activator and an inhibitor, respectively. We suppose the activator diffuses slowly and the inhibitor diffuses rapidly, that is \(D_v \ll D_u\). The spatial pattern generated by (2.21) is shown in Figure 2.1. It is assumed that a change in cells or tissue takes place in the region where the activator concentration is high. They used this system to simulate the regeneration and transplantation experiments on hydra. Hydra is an animal with body length of a few millimeters. If the head is amputated, then a new head regenerates within a few days. When the head is removed, the head-activating substance represented by \(u\) is released from cells, and activation proceeds by mechanism in which the released substances themselves influence further release. The results with localized pattern of the activator concentration as in Figure 2.1 are in agreement with experiments.

3. Lengyel–Epstein Model

In this section, we demonstrate how a stable steady state loses its stability and spatially inhomogeneous patterns can emerge. We use the Lengyel–Epstein model, which is a typical and important example which gives rise to the Turing instability:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= D_1 \frac{\partial^2 u}{\partial x^2} - u - \frac{4uv}{1+u^2} + a, & 0 < x < L, t > 0, \\
\frac{\partial v}{\partial t} &= \delta \left[ D_2 \frac{\partial^2 v}{\partial x^2} + b \left( u - \frac{uv}{1+u^2} \right) \right], & 0 < x < L, t > 0, \\
\frac{\partial u}{\partial x} &= \frac{\partial v}{\partial x} = 0, & x \in [0, L], t > 0,
\end{align*}
\]
where $D_1$, $D_2$, $a$, $b$, $\delta$ are positive constants. In the following, we use $a = 30$, $b = 2.8$, $\delta = 8$ for the sake of convenience.

The Lengyel–Epstein model is an activator-inhibitor system, where $u = u(x,t)$ represents the concentration of an activator, $v = v(x,t)$ represents the concentration of an inhibitor. We study only positive solutions of (3.1). The corresponding system of ordinary differential equations of is given by

$$
\begin{align*}
\frac{du}{dt} &= -u - \frac{4uv}{1 + u^2} + a, \\
\frac{dv}{dt} &= \delta b \left( u - \frac{uv}{1 + u^2} \right).
\end{align*}
$$

(3.2)

First, we find steady-state solutions of (3.2). Letting $f(u,v) = -u - \frac{4uv}{1 + u^2} + a$, $g(u,v) = \delta b \left( u - \frac{uv}{1 + u^2} \right)$, we solve $f(u,v) = 0$ and $g(u,v) = 0$. We see that (3.2) has only one equilibrium point $(\bar{u}, \bar{v})$ in the first quadrant of $uv$-plane (see Figure 3.1), which is

$$(\bar{u}, \bar{v}) = \left( \frac{a}{3} \cdot 1 + \frac{a^2}{25} \right) = (6, 37).$$

Next, we check the stability of the equilibrium $(\bar{u}, \bar{v})$. Since we use the linearization of system (3.2) at $(\bar{u}, \bar{v})$, let $u(t) = \bar{u} + \psi(t)$, $v(t) = \bar{v} + \epsilon v(t)$.

Then, we obtain the linearized system of (3.2) at $(\bar{u}, \bar{v})$:

$$
\frac{d}{dt} \begin{pmatrix} \phi \\ \psi \end{pmatrix} = \begin{pmatrix} -1 - \frac{4(1 - \bar{u}^2)}{1 + \bar{u}^2} & -\frac{4\bar{u}}{1 + \bar{u}^2} \\ \delta b & -\delta b \frac{\bar{u}}{1 + \bar{u}^2} \end{pmatrix} \begin{pmatrix} \phi \\ \psi \end{pmatrix}.
$$

We study the signs of the real parts of eigenvalues of the matrix on the right-hand side above. If $(\bar{u}, \bar{v})$ is asymptotically stable, then it is satisfied

$$f_a + g_c < 0 \quad \text{and} \quad f_a g_c - f_c g_a > 0.$$

Therefore, we have

$$-1 - \frac{4(1 - \bar{u}^2)}{1 + \bar{u}^2} - \delta b \frac{\bar{u}}{1 + \bar{u}^2} < 0,$$

(3.3)
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The solution, which is given by

\[ s = \frac{1}{2} \left( 1 - \sqrt{1 - 4\delta b (1 - \frac{\tilde{u}}{1 + \tilde{u}^2})} \right) \]

for \((\tilde{u}, \tilde{v})\) is stable. It turns out that both (3.3) and (3.4) are satisfied when \(\tilde{u} = 6, b = 2.8, \delta = 8\). Hence, the unique equilibrium point \((\tilde{u}, \tilde{v}) = (6, 37)\) of (3.2) is asymptotically stable.

In order to obtain Turing patterns, the stable equilibrium \((\bar{u}, \bar{v})\) of (3.2) has to be destabilized in (3.1) with unequal diffusions. To see it, we study eigenvalues of a linearized operator of (3.1). We substitute the functions

\[ u(x, t) = \tilde{u} + \varepsilon(x, t), \quad v(x, t) = \tilde{v} + \varepsilon v(x, t) \]

into (3.1) to obtain the linearized system of (3.1) at \((\tilde{u}, \tilde{v})\):

\[
\frac{\partial}{\partial t} \begin{pmatrix} z \\ w \end{pmatrix} = \begin{pmatrix} D_1 \frac{\partial^2 z}{\partial x^2} - 1 - \frac{4(1 - \tilde{v})}{1 + \tilde{v}^2} & -\frac{4\tilde{u}}{1 + \tilde{v}^2} \\ \delta b \left( 1 - \frac{1 - \tilde{u}}{1 + \tilde{u}^2} \right) & \delta D_2 \frac{\partial^2 w}{\partial x^2} - \frac{\tilde{u}}{1 + \tilde{u}^2} \end{pmatrix} \begin{pmatrix} z \\ w \end{pmatrix}.
\]

We express the functions \(z\) and \(w\) in terms of trigonometric series (2.12). Substitute these expansions into the linearized equation above and compare the coefficients of \(\frac{\partial^n}{\partial x^n} x\) on the both sides to obtain, for \(n = 0, 1, 2, \ldots\),

\[
\frac{d}{dt} \begin{pmatrix} z_n \\ w_n \end{pmatrix} = \begin{pmatrix} -D_1 \left( \frac{\pi n}{L} \right)^2 - 1 - \frac{4(1 - \tilde{v})}{1 + \tilde{v}^2} & -\frac{4\tilde{u}}{1 + \tilde{v}^2} \\ \delta b \left( 1 - \frac{1 - \tilde{u}}{1 + \tilde{u}^2} \right) & -\delta D_2 \left( \frac{\pi n}{L} \right)^2 - \frac{\tilde{u}}{1 + \tilde{u}^2} \end{pmatrix} \begin{pmatrix} z_n \\ w_n \end{pmatrix}.
\]

It follows from \(D_1 > 0, D_2 > 0\) and (3.3) that the following inequality always holds:

\[-D_1 \left( \frac{\pi n}{L} \right)^2 - 1 - \frac{4(1 - \tilde{v})}{1 + \tilde{v}^2} - \delta D_2 \left( \frac{\pi n}{L} \right)^2 - \delta b - \frac{\tilde{u}}{1 + \tilde{u}^2} < 0.\]

Therefore, \((\bar{u}, \bar{v})\) becomes an unstable stationary solution of (3.1) if and only if there exists an \(n \geq 1\) such that

\[-D_1 \left( \frac{\pi n}{L} \right)^2 - 1 - \frac{4(1 - \tilde{v})}{1 + \tilde{v}^2} - \delta D_2 \left( \frac{\pi n}{L} \right)^2 - \delta b - \frac{\tilde{u}}{1 + \tilde{u}^2} < 0.\]

Thus, after some calculations, we obtain the following inequality:

\[ D_1 < \frac{L^2}{(\pi n)^2} \left[ 4(\tilde{u}^2 - 1) - 1 - \frac{L^2 8b\tilde{u}^3}{(\tilde{u}^2 + 1)(D_2(\pi n)^2(\tilde{u}^2 + 1) + L^2 b\tilde{u})} \right]. \]

For any fixed \(D_2\), if the right-hand side of (3.6) is positive for some \(n \geq 1\), then \((\bar{u}, \bar{v})\) becomes unstable for \(D_1\) sufficiently small. Then, a spatial pattern of mode \(n\) is expected to appear. The integer \(n\) determines the spatial period \(\omega\) of the solution, which is given by \(\omega = 2\pi/n\). Let us study it more precisely.
For each \( n/C_21 \geq 1 \), we draw a graph of the following equation in the first quadrant of \( D_2/D_1 \)-plane:
\[
D_1 = \frac{L^2}{(\pi n)^2} \left[ \frac{4(\bar{u}^2 - 1)}{\bar{u}^2 + 1} - 1 - \frac{L^2 b\bar{u}^3}{(\bar{u}^2 + 1)(D_2(\pi n)^2(\bar{u}^2 + 1) + L^2 b\bar{u})} \right].
\]
(3.7)

In Figure 3.2, each curve approaches \( D_1 = \frac{L^2}{(\pi n)^2} \left( \frac{4(\bar{u}^2 - 1)}{\bar{u}^2 + 1} - 1 \right) \) as \( D_2 \to +\infty \). The abscissa of this asymptote tends to 0 as \( n \to +\infty \). Each curve intersects the \( D_2 \)-axis at
\[
D_2 = \frac{L^2 b\bar{u}}{(\pi n)^2(3\bar{u}^2 - 5)}.
\]
and this intersection moves to the origin as \( n \to +\infty \).

For each \( n \geq 1 \), we draw a graph of the following equation in the first quadrant of \( D_2/D_1 \)-plane:
\[
D_1 = \frac{L^2}{(\pi n)^2} \left[ \frac{4(\bar{u}^2 - 1)}{\bar{u}^2 + 1} - 1 - \frac{L^2 b\bar{u}^3}{(\bar{u}^2 + 1)(D_2(\pi n)^2(\bar{u}^2 + 1) + L^2 b\bar{u})} \right].
\]
(3.7)

Letting \( L = 10 \), we shall observe the mechanism of the Turing instability, and see how Turing patterns emerge by numerical simulations. For fixed \( D_2 = 1.5 \), we use \( D_1 \) as a parameter to obtain the diffusion driven instability. Figure 3.4 is focused on the intersection of curves \( n = 3 \) and \( n = 4 \). The value of \( D_1 \) corresponding to the intersections of the curves \( n = 3 \) and \( n = 4 \) is 1.011822867 \( \cdots \). The yellow star in Figure 3.3 denotes a point with \( D_1 = 0.95 \), which is above the curve \( n = 3 \), while it is below the curve \( n = 4 \). This means that \((\bar{u}, \bar{v})\) does not lose its stability against the
spatial perturbation of mode \( n = 3 \). On the other hand, it is destabilized by the spatial perturbation of mode \( n = 4 \).

Therefore, it is expected that if we take \( D_1 = 0.95 \) and \( D_2 = 1.5 \), then small perturbations to \((\tilde{u}, \tilde{v})\) grow and a spatial pattern with mode \( n = 4 \) emerges. Indeed, it can be demonstrated by numerical simulations, see Figure 3.5.

Now, let \( D_1 = 1.5 \) and \( D_2 = 1.5 \). This case is marked by the pink disk in Figure 3.4. We solve (3.1) numerically, choosing a spatial pattern with mode \( n = 4 \) as its initial data. Since the condition where \( D_1 = 1.5 \) and \( D_2 = 1.5 \) is above the curve \( n = 4 \), the constant solution \((\tilde{u}, \tilde{v})\) is not destabilized by this spatial mode. Therefore, we can see in Figure 3.6 that a solution starting from the pattern with mode \( n = 4 \) comes back to \((\tilde{u}, \tilde{v})\).
4. Discrete Models

Cellular automata are theoretical models which consist of a regular grid of cells. Each cell is in one of a finite number of states such as {green, red, yellow}. For each cell, a set of cells called “neighborhood” is defined relatively to a specified cell. If a fixed rule is given and an initial condition is selected by assigning a state for each cell, a new state of each cell is determined by the current state of the cell and the states of cells in its neighborhood. In Figure 4.1, where a one-dimensional grid of finitely many cells is considered and each line denotes the states of cells at time $t_i$, it is illustrated that two waves propagate and they retain their forms after collision. The rule to determine a state at time $t$ is as follows: for each cell from left to right at each state,

- if a cell is empty and you have balls, you put a ball into the cell,
- if a cell is empty and you have no ball, then nothing should be done for the cell, and you go to the next cell,
- if there is a ball in a cell, you remove it from the cell and carry it,
- if you have come to the end of the state (the right-hand side), you go to the next time step $t + 1$.

In Figure 4.1, the top line shows the initial state ($t = 0$), and you start without balls in your hand. The second line and below show the subsequent development.

Cellular automata exhibit the complex behavior from quite simple rules. Therefore, they have been widely investigated in physics, chemistry, biology and computer sciences. In the pattern formation, a cellular automaton simulates the BZ reaction which creates self-organized target patterns or spiral waves in a thin unstirred layer of a reaction solution. Moreover, Turing patterns can be explained by some cellular automata. It is known that patterns on some seashell (Figure 5.1) are simulated by cellular automata following simple rules. It is an interesting problem to understand the relation between reaction-diffusion models (continuous models) and cellular automata.

In this section, we show how to derive nonlinear difference–difference equations from nonlinear differential equations taking the Lotka–Volterra equations as examples.

4.1 Lotka–Volterra equations

The Lotka–Volterra equations are nonlinear differential equations describing the dynamics of the growth of two populations, one a predator and the other a prey:

\[
\begin{align*}
\frac{du}{dt} &= (\beta - v)u, \\
\frac{dv}{dt} &= (u - \alpha)v,
\end{align*}
\]

where $\alpha$ and $\beta$ are positive constants. The function $u = u(t)$ is the density of prey and $v = v(t)$ is the density of predator. Let

\[ V = V(u, v) = u + v - \alpha \log u - \beta \log v. \]
A direct calculations shows that \( V(t) = 0 \) which implies that \( V \) is a conserved quantity for system (4.1). Therefore, solution orbits for (4.1) correspond level curves of \( V \), see Figure 4.2. In Figure 4.3, the progression of two species over time is plotted. The Lotka–Volterra equations can be generalized to systems of more than two species. Let \( X_j \) be a species at time \( t \) and \( u_j(t) \) be its population density. Assuming \( X_j \) preys on \( X_{j-1} \) and \( X_{j+1} \) is its predator, we obtain, for each \( j \), the following equations:

\[
\frac{du_j}{dt} = u_j(u_{j-1} - u_{j+1}).
\] (4.2)

Here, all parameters were set 1, for simplicity.

Suppose there are only four species \( X_0, X_1, X_2, X_3 \) and the numbers of \( X_0 \) and \( X_3 \) are constants, that is, \( u_0(t) = a, u_3(t) = b \) for some \( a > 0 \) and \( b > 0 \). Then, the dynamics of \( X_1 \) and \( X_2 \) is given by the system

\[
\frac{du_1}{dt} = u_1(a - u_2),
\]
\[
\frac{du_2}{dt} = u_2(u_1 - b),
\]

which is exactly the same as (4.1). Therefore, (4.1) is a special case of the generalized system (4.2). Hereafter, we call (4.2) the Lotka–Volterra system, and let \(-\infty < j < +\infty\).

4.2 Problems caused by nonlinearity

In general, it is difficult to expect that there is an explicit formula of solutions to nonlinear differential equations. In such a case, numerical simulations are helpful in understanding the dynamics of solutions. We want to believe that numerical simulations give us good approximations to solutions of reaction-diffusion systems. But a nonlinearity sometimes causes strange or unusual behavior of solutions.

The Lorenz oscillator is one of the examples which exhibit chaotic behavior. The Lorenz oscillator is a nonlinear three-component dynamical system:

\[
\begin{align*}
\frac{du}{dt} &= -pu + py, \\
\frac{dv}{dt} &= -uv + ru - v, \\
\frac{dw}{dt} &= uv - bw.
\end{align*}
\] (4.3)

Here, \( p, r, b \) are positive constants. Figures 4.4 and 4.5 show the behavior of solutions of (4.3) starting from a slightly different initial data. They are calculated for the same values of the parameters \( p, r, b \) and the same time interval. It is observed that the two orbits do not look close to each other.
4.3 Finite difference methods

In the one-dimensional case, a finite difference method is a fundamental way to approximate a solution of differential equations. First, the space-time plane is divided into a uniform grid. Let the mesh size of the x-axis be $h$ and that of the $t$-axis be $k$. We consider the following reaction-diffusion equation:

$$
\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + f(u) \quad \text{for } 0 < x < 1, 0 < t < T
$$

(4.4)

associated with the non-flux boundary condition and the initial condition:

$$
\begin{align*}
\frac{\partial u}{\partial x}(0, t) &= \frac{\partial u}{\partial x}(1, t) = 0 \quad \text{for } t > 0, \\
u(x, 0) &= u_0(x) \quad \text{for } 0 < x < 1.
\end{align*}
$$

(4.5)

(4.6)

Here, $u = u(x, t)$ represents the concentration of a chemical substance, and $f(u)$ is a nonlinear term, for example, $f(u) = u^2$. The initial data $u_0(x)$ is a given function. The approximation of a solution $u(x, t)$ of (4.4) at point $x_j = jh$ and at time $t = nk$ is denoted by $u^n_j$ for $0 \leq j \leq J$ and $0 \leq n \leq N$. There are two examples of finite difference schemes:

**explicit method:**

$$
\frac{u^{n+1}_j - u^n_j}{k} = \frac{u^n_j - 2u^n_{j+1} + u^n_{j-1}}{h^2} + (u^n_j)^2,
$$

(4.7)

**implicit method:**

$$
\frac{u^{n+1}_j - u^n_j}{k} = \frac{u^{n+1}_{j+1} - 2u^{n+1}_{j} + u^{n+1}_{j-1}}{h^2} + (u^{n+1}_j)^2.
$$

(4.8)

On the boundary, $u^n_0$ and $u^n_J$ for $0 \leq n \leq N$ are replaced by $u^n_0$ and $u^n_{J-1}$, respectively. In the explicit method (4.7), we obtain the values of $u^{n+1}_j$, $0 \leq j \leq J$, immediately if the values at time $n$ are given. On the other hand, the implicit method (4.8) requires to solve a system of numerical equations on each time step.

Let $u(x, t)$ be an exact solution of (4.4) with initial data $\phi(x)$, and $u^n_j$ for $0 \leq j \leq J$, $0 \leq n \leq N$ be a solution of a discretized equation of (4.4) with initial data $\phi_j$. Here, $\phi_j$ means the value of $\phi(x)$ at $x = jh$. For the moment, we assume that $f(u) \equiv 0$ in (4.4) and consider the linear diffusion equation. Let $m$ be an arbitrary positive integer and let us study how the amplitude behaves for the specific initial data $\phi_j = \sin(\pi m(jh))$ with $0 \leq j \leq J$. For this purpose, we put $u^n_j = A_n X_j$, where $X_j = \sin(\pi m(jh))$, and substitute these in (4.7). Then, we have

$$
A_{n+1} = (1 - 2\lambda + 2\lambda \cos(\pi mh))A_n.
$$

If the sequence $(A_n)_{n=0}^\infty$ remains bounded for any positive integer $m$, then the scheme is said to be *stable*. Clearly, the explicit scheme is stable if and only if $\lambda \leq 1/2$. On the other hand, if we substitute $u^n_j = A_n X_j$ in (4.8), then we obtain

$$(1 + 2\lambda - 2\lambda \cos(\pi mh))A_{n+1} = A_n.
$$

Since $1 + 2\lambda(1 - \cos(\pi mh)) \geq 1$ for any positive integer $m$, we see that $(A_n)_{n=0}^\infty$ is bounded for any $m$ no matter how $\lambda > 0$ is. In this case, the implicit scheme (4.8) is *unconditionally stable*.

The error in a solution of a discretized equation is defined as the difference between its approximation and the exact solution of differential equation. There are two sources of errors. One is called a round-off error, which is the loss of precision due to rounding of decimals in computers. The other is called a discretization error, which is the difference between the solution of the discretized equation and the exact solution of the original differential equation. In general, it
is not expected to obtain the formula for exact solutions of nonlinear differential equations. Then, it is difficult to estimate the difference between solutions of discretized equations and original differential equations. Moreover, as it is seen in the Lorenz equations, the discretization error can lead to unexpected behavior of solutions to nonlinear differential equations. Therefore, we have to pay attention to what numerical simulations explain, and to what we can and cannot understand through them.

Recently, much attention has been focused on numerical schemes that conserve the structure of the solution set. Such schemes have been developed to study e.g. integrable nonlinear equations, describing the propagation of soliton. A soliton is a solitary wave which keeps its form after collision. The KdV equation and the nonlinear Schrödinger equation are examples of soliton equations. Moreover, the generalized Lotka–Volterra equations (4.2) also have soliton solutions. The structure-conserving numerical schemes are required to preserve such a quality of soliton after discretizing differential equations.

In the following, we introduce one of the methods for deriving a finite difference scheme which keeps its conserved quantity. Using the Lotka–Volterra equation (4.2) as an example, we show how to construct a discrete equation which keeps solitons. On the basis of this idea, we would like to understand a connection between reaction-diffusion equations and cellular automata in the last part of this section.

4.4 Bilinearization methods

In this and next subsections, we describe methods which are introduced in [5, 6]. We discretize the Lotka–Volterra equation (4.2) in the following three steps:

1. transform (4.2) into a bilinear differential equation, where the resulting equation is invariant under gauge transformations;
2. derive a discrete bilinear equation which keeps the gauge invariance;
3. obtain a discrete equation from the discrete bilinear equation.

Let \( x(t) \) be a solution of a differential equation. The gauge transformation is defined by changing the dependent variable \( x(t) \) to \( x(t)g(t) \) for an arbitrary function \( g(t) \) of \( t \). If the differential equation for \( x \) is invariant under gauge transformation, then it is said to be gauge invariant.

We shall obtain a discrete Lotka–Volterra equation from (4.2) following those three steps above. Here, we write (4.2) again:

\[
\frac{du_j}{dt} = u_j(u_{j-1} - u_{j+1}),
\]

where \( u_j(t) \) is the number of species \( X_j \) at time \( t \). We impose boundary conditions \( u_j(t) \to 1 \) as \( j \to \pm\infty \) on (4.2).

**Step 1: From nonlinear differential equations to bilinear differential equations.** Introducing new variables \([f_j(t)]\), we assume that \( u_j \) is expressed as follows:

\[
u_j = \frac{f_{j-1}f_{j+2}}{f_j f_{j+1}}.
\]  (4.9)
In addition, on $f_j$’s imposed are boundary conditions $f_{j+1}/f_j \to c_\pm$ as $j \to \pm\infty$. Here, $c_+$ (or $c_-$) is a constant independent of $j$ and $t$. These boundary conditions for $f_j$ are natural. Indeed, since $u_j(t) \to 1$ as $j \to \pm\infty$, it follows from (4.9) that $f_j$ should satisfy $f_{j+2}/f_j = f_j/f_{j-1}$ as $j \to \pm\infty$.

Substituting (4.9) into (4.2) leads to the following bilinear differential equation

$$f_{j+1} \frac{df_j}{dt} - f_j \frac{df_{j+1}}{dt} = f_{j-1}f_{j+2} - f_jf_{j+1}. \quad (4.10)$$

Indeed, dividing both sides of (4.2) by $u_j$, we obtain

$$\frac{d\log u_j(t)}{dt} = u_{j-1} - u_{j+1}.$$ 

Substituting (4.9) into the left-hand side above, we have

$$\frac{d\log u_j(t)}{dt} = \frac{d}{dt} \log \left| \frac{f_{j-1}f_{j+2}}{f_jf_{j+1}} \right| = \frac{d}{dt} \log \left| \frac{f_{j-1}}{f_j} \right| + \frac{d}{dt} \log \left| \frac{f_{j+2}}{f_{j+1}} \right|.$$ 

This implies, for all $j$, that

$$\frac{d}{dt} \log \left| \frac{f_{j+2}}{f_{j+1}} \right| + u_{j+1} = -\frac{d}{dt} \log \left| \frac{f_{j-1}}{f_j} \right| + u_{j-1}$$

$$= \frac{d}{dt} \log \left| \frac{f_{j-1}}{f_j} \right|^{-1} + u_{j-1}$$

$$= \frac{d}{dt} \log \left| \frac{f_{j}}{f_{j-1}} \right| + u_{j-1}. \quad (4.11)$$

By induction on $j$ we find that the right-hand side is equal to

$$\frac{d}{dt} \log \left| \frac{f_{j-m}}{f_{j-m-1}} \right| + u_{j-m-1}$$

for all positive integer $m$. Then, it follows from the boundary condition for $f_j$ that the right-hand side of (4.11) tends to 1 as $j \to -\infty$ (assuming that $f_{j+1}/f_j$ is convergent together with its derivative). Hence, we see, for all $j$, that

$$\frac{d}{dt} \log \left| \frac{f_{j+1}}{f_j} \right| + \frac{f_{j-1}f_{j+2}}{f_jf_{j+1}} = 1.$$ 

After direct calculations, we get

$$\frac{1}{f_{j+1}} \frac{df_{j+1}}{dt} = \frac{1}{f_j} \frac{df_j}{dt} + \frac{f_{j-1}f_{j+2}}{f_jf_{j+1}} = 1,$$

which implies (4.10).

The bilinear differential equation (4.10) has the gauge invariance. To see this, transform $f_j$ to $g(t)f_j(t)$ for $l = j - 1, j + 1, j - 2$ and compute

$$g f_{j+1} \frac{dg_{j+1}}{dt} - (g_{j+1}) \frac{dg_j}{dt} - (g_{j+1}) (g_{j+2}) - (g_j) (g_{j+1})$$

$$= g f_{j+1} \left( \frac{df_j}{dt} + g \frac{df_{j+1}}{dt} \right) - g f_j \left( \frac{df_{j+1}}{dt} + g \frac{df_{j+2}}{dt} \right) - g^2 (f_{j-1}f_{j+2} - f_jf_{j+1})$$

$$= g^2 \left( \frac{df_{j+1}}{dt} - f_j \frac{df_{j+1}}{dt} \right) - g^2 (f_{j-1}f_{j+2} - f_jf_{j+1}).$$

Therefore, if the $f_j$’s satisfy (4.10), so do the $g f_j$’s.

**Step 2:** From bilinear differential equations to discrete bilinear equations. Our goal is to obtain a discrete equation for (4.2) which has conserved quantities. To do so, we first derive a discrete bilinear equation from (4.10).

If we discretize (4.10) by the explicit scheme, then we have

$$f_{j+1}(t) \left( \frac{f_j(t+k) - f_j(t)}{k} \right) - f_j(t) \left( \frac{f_{j+1}(t+k) - f_{j+1}(t)}{k} \right) = f_{j-1}(t)f_{j+2}(t) - f_j(t)f_{j+1}(t), \quad (4.12)$$

where $k$ is the mesh size of time interval. It is easy to see that (4.12) does not have any gauge invariance. Indeed, if we replace $f_j(t)$ by $g(t)f_j(t)$ in (4.12), then

$$g(t) g(t+k) \left( \frac{f_{j+1}(t)f_j(t+k)}{k} - \frac{f_j(t)f_{j+1}(t+k)}{k} \right) = g^2 (f_{j-1}(t)f_{j+2}(t) - f_j(t)f_{j+1}(t)),$$

which is not satisfied unless $g(t+k) = g(t)$. Hence, (4.12) is not invariant under gauge transformations.
Since we want (4.12) to have the gauge invariance, we shift the time variable on the right-hand side of (4.12) to obtain
\[
f_{j+1}(t) \frac{f_j(t+k) - f_j(t)}{k} = f_j(t) \frac{f_{j+1}(t+k) - f_{j+1}(t)}{k} = f_{j-1}(t) f_{j+2}(t+k) - f_j(t+k) f_{j+1}(t).
\] (4.13)

Let \( t = nk \) and denote \( f(nk) \) by \( f^n \). Then, equation (4.13) can be rewritten as
\[
(1 + k) f^n_{j+1} f^n_{j+1} = f^n_{j+1} f^n_{j+1} + k f^n_{j-1} f^n_{j+2}.
\] (4.14)

This is the desired discrete bilinear equation for (4.10).

**Step 3: From discrete bilinear equation to discrete Lotka–Volterra equations.** Finally, we obtain a discrete Lotka–Volterra equation from (4.14). To come back to the variable \( u^n_i \) from \( f^n_i \), we set
\[
u^n_i = \frac{f^n_{i-1} f^n_{i+2}}{f^n_i}.
\] (4.15)

Then, we have
\[
u^n_{j+1} \quad \frac{\nu^n_j}{\nu^n_i} = \frac{f^n_{j-1} f^n_{j+2} f^n_{j+1}}{f^n_{j+1} f^n_{j+2} f^n_{j-1} f^n_{j+2}},
\] (4.16)

Since
\[
u^n_{j+1} \quad \frac{\nu^n_j}{\nu^n_i} = \frac{f^n_{j-2} f^n_{j+1}}{f^n_{j-1} f^n_{j+2}},
\]

we see that identity (4.16) becomes
\[
u^n_{j+1} \quad \frac{\nu^n_j}{\nu^n_i} = \frac{f^n_{j-1} f^n_{j+2} f^n_{j+1}}{f^n_{j+1} f^n_{j+2} f^n_{j-2}}.
\] (4.17)

From (4.14), the following two equations hold:
\[
(1 + k) f^n_{j+1} f^n_{j+2} = f^n_{j+1} f^n_{j+2} + k f^n_{j+1} f^n_{j+3},
\] (4.18)
\[
(1 + k) f^n_{j+1} f^n_{j} = f^n_{j+1} f^n_{j+1} + k f^n_{j-2} f^n_{j+1}.
\] (4.19)

Substituting (4.18) into the right-hand side of (4.17), we obtain
\[
u^n_{j+1} \quad \frac{\nu^n_j}{\nu^n_i} = \frac{(1 + k) f^n_{j+2} f^n_{j} u^n_{j-1}}{f^n_{j+1} f^n_{j+2} f^n_{j-2}} (1 + k f^n_{j+1} f^n_{j+3}) = \frac{(1 + k) f^n_{j+1} f^n_{j} u^n_{j-1}}{f^n_{j+1} f^n_{j+2} f^n_{j-2}}(1 + k u^n_{j+1})
\] (4.20)

Furthermore, it follows from (4.19) that
\[
(1 + k) f^n_{j+1} f^n_{j+1} = f^n_{j+1} f^n_{j+1} + k.
\] Therefore, substituting the above equation into the right-hand side of (4.20) gives
\[
u^n_{j+1} \quad \frac{\nu^n_j}{\nu^n_i} = \frac{u^n_{j-1}}{1 + k u^n_{j+1}} (f^n_{j+1} f^n_{j} + k).
\] (4.21)

Since \((f^n_{j+1} f^n_{j})/(f^n_{j+2} f^n_{j+1}) = (u^n_{j-1})^{-1}\), we see
\[
u^n_{j+1} \quad \frac{\nu^n_j}{\nu^n_i} = \frac{1 + k u^n_{j-1}}{1 + k u^n_{j+1}}.
\] (4.22)

Consequently, the following discrete Lotka–Volterra equation is obtained:
\[
u^n_{j+1} \quad \frac{\nu^n_j}{\nu^n_i} = u^n_{j-1} u^n_{j+1} u^n_{j+1}.
\] (4.23)

In the following, we shall see that equation (4.23) has a soliton solution which is given by formula (4.42) below and the transformation (4.15).

We have introduced the procedure to obtain a discrete Lotka–Volterra equation which has conserved quantities. This reasoning seems to be complicated because of several calculations and it is not easy to solve (4.23). However, it is important to have this relation in order to introduce the corresponding cellular automata.
4.5 Ultradiscretization methods

Cellular automata are discrete dynamical systems that consist of a lattice of discrete identical cells. The states of cells evolve in discrete time steps according to simple rules. Note that dependent variables of this system are discrete. On the other hand, dependent variables of difference equations are still continuous quantities though they are considered in the space-time plane which is divided into a uniform grid. For example, \( u_j^n \) in (4.23) represents the density of the species \( X_j \) at point \( x_j = jh \) and at time \( t = nk \), where \( h \) and \( k \) are the mesh size of space and time, respectively. Here, the word “density” suggests that the state varies continuously, not discretely.

In the following, we introduce a technique to discretize dependent variables of differential equations, and we relate differential equations with cellular automata.

4.5.1 Ultradiscrete diffusion equations

First, we obtain the discrete counterpart of the following diffusion equation in one-dimensional space:

\[
\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2},
\]

(4.24)

where \( u = u(x, t) \) represents the density of particles. Let the space and time variables be divided by \( N \), and let \( h = 1/N \) and \( k = T/N \). We denote the value of \( u(x, t) \) at point \( x_j = jh \) and time \( t = nk \) by \( u_j^n \). Using the explicit method (4.7), we have

\[
u_j^{n+1} = u_j^n + \frac{k}{h^2} (u_{j-1}^n - 2u_j^n + u_{j+1}^n),
\]

(4.25)

where the dependent variable has not been discretized yet. In the following, we put \( k/h^2 = 1/2 \) for simplicity, which assures us that (4.27) is obtained.

Assume \( u_j^n \leq u_{j+1}^n \) for all \( 0 \leq j \leq N \) at time \( n \). We note that the particles diffuse from the place of higher density to that of lower. If

\[
\cdots = u_{j-2}^n = u_{j-1}^n < u_j^n = u_{j+1}^n = \cdots,
\]

(4.26)

then diffusion occurs left from \( u_j^n \) but it never occurs from \( u_{j+1}^n \) to \( u_j^n \). Since the state between \( u_{j+1}^n \) and \( u_j^n \) will be in equilibrium, the next time step becomes

\[
u_{j-2}^{n+1} < u_{j-1}^{n+1} = u_j^{n+1} < u_{j+1}^{n+1}.
\]

(4.27)

Introduce new variable \( V_j^n \) as follows. If \( u_j^n = u_{j+1}^n \), then there is no diffusion effect from right to left. We denote this state by \( V_j^n = 0 \). If \( u_j^n < u_{j+1}^n \), then the diffusion occurs from right to left. This is the state \( V_j^n = 1 \). Hence, the example (4.26) above shows that \( V_{j-1}^n = 1 \) and \( V_j^n = 0 \) becomes \( V_{j-1}^{n+1} = 0 \) and \( V_j^{n+1} = 1 \). As a result, the dependent variable in (4.25) has been discretized. This kind of discretizing process on a dependent variable is called ultradiscretization. We now start to derive an ultradiscretization from the diffusion.

Introducing a new variable \( v_j^n \) defined by

\[
v_j^n = \frac{1}{h} \frac{u_{j+1}^n}{u_j^n},
\]

(4.28)

we will obtain a discrete equation for \( v_j^n \). Since

\[
\frac{v_j^{n+1}}{v_j^n} = \frac{u_{j+1}^{n+1} u_j^n}{u_{j+1}^{n+1} u_{j+1}^{n+1}},
\]

and it follows from (4.25) that

\[
\frac{u_j^{n+1}}{u_j^n} = 1 - 2 \frac{k}{h^2} \frac{u_j^n}{h^2} \frac{u_{j+1}^n}{u_j^n},
\]

\[
\frac{u_{j+1}^{n+1}}{u_{j+1}^n} = 1 - 2 \frac{k}{h^2} \frac{u_{j+1}^n}{h^2} \frac{u_{j+2}^n}{u_{j+1}^n}.
\]

Thus, we have

\[
v_j^{n+1} = 1 - 2 \frac{k}{h^2} \frac{u_j^n + u_{j+2}^n}{h^2} \frac{u_{j+1}^n}{u_j^n},
\]

(4.29)

From the definition of \( v_j^n \), equation (4.29) becomes
Furthermore, we transform $v_j^p$ into

$$v_j^p = e^{v_j^p/\varepsilon}$$

for $\varepsilon > 0$, and assume $h$ and $k$ satisfy

$$h^2 = e^{-1/\varepsilon},$$

$$h^3 - 2h = e^{-1/\varepsilon}.$$  (4.32)

Substituting (4.31) into (4.30), we obtain

$$e^{v_j^p+1/\varepsilon} = e^{v_j^p/\varepsilon} \frac{1 - 2 \frac{k}{h^3} + \frac{k}{h^2} (e^{-V_j^p/\varepsilon} + h^2 e^{V_j^p+1/\varepsilon})}{1 - 2 \frac{k}{h^3} + \frac{k}{h^2} (e^{-V_j^p/\varepsilon} + h^2 e^{V_j^p+1/\varepsilon})}.$$  (4.33)

Relation (4.33) leads to the identity

$$1 - 2 \frac{k}{h^3} = \frac{k}{h^3} \left( \frac{h^3}{k} - 2h \right) = \frac{k}{h^3} e^{-1/\varepsilon},$$

which, together with (4.32), allows us to transform (4.31) as follows

$$e^{v_j^p+1/\varepsilon} = e^{v_j^p/\varepsilon} e^{-1/\varepsilon} + e^{v_j^p/\varepsilon} + e^{(V_j^p+1)/\varepsilon}$$

$$e^{-1/\varepsilon} + e^{V_j^p+1/\varepsilon}.$$  (4.34)

Computing the logarithms of both sides of (4.34), we see

$$V_j^{p+1} = V_j^p + \varepsilon \log[e^{-1/\varepsilon} + e^{V_j^p/\varepsilon} + e^{(V_j^p+1)/\varepsilon}] - \varepsilon \log[e^{-1/\varepsilon} + e^{V_j^p+1/\varepsilon} + e^{(V_j^p+1)/\varepsilon}].$$  (4.35)

Now, we need the following lemma to connect (4.35) with a cellular automaton.

**Lemma 4.1.** The following identity holds:

$$\lim_{\varepsilon \to +0} \varepsilon \log(e^{A/\varepsilon} + e^{B/\varepsilon}) = \max(A, B),$$

for all $A > 0$ and $B > 0$.

**Proof.** First, assume that $A > B$. Then, the left-hand side of (4.36) is

$$\lim_{\varepsilon \to +0} \varepsilon \log[e^{A/\varepsilon} (1 + e^{-(A-B)/\varepsilon})] = A + \lim_{\varepsilon \to +0} \varepsilon \log(1 + e^{-(A-B)/\varepsilon}).$$

Since $A - B > 0$, the limit on the right-hand side above is equal to 0. This shows (4.36). The case $B > A$ can be proved by the same argument.

Next, assume $A = B$. It is easy to see that the left-hand side of (4.36) satisfies

$$\lim_{\varepsilon \to +0} \varepsilon \log 2 e^{A/\varepsilon} = A + \lim_{\varepsilon \to +0} \varepsilon \log 2 = A.$$  

\[\square\]

**Remark 4.2.** By virtue of Lemma 4.1, the following general formula holds:

$$\lim_{\varepsilon \to +0} \varepsilon \log(e^{A_1/\varepsilon} + e^{A_2/\varepsilon} + \ldots + e^{A_n/\varepsilon}) = \max(A_1, A_2, \ldots, A_n).$$  (4.37)

Now, let us come back to the estimate of (4.35) by making use of Lemma 4.1. Computing the limits as $\varepsilon \to +0$ of both sides of (4.35), we obtain

$$V_j^{p+1} = V_j^p + \max(-1, -V_j^p, -(1 - V_{j+1}^p)) - \max(-1, -V_{j-1}^p, -(1 - V_{j}^p)).$$

Note that $\min(A, B) = -\max(-A, -B)$. Therefore, we get the ultradiscrete diffusion equation

$$V_j^{p+1} = V_j^p - \min(1, V_j^p, 1 - V_{j+1}^p) + \min(1, V_{j-1}^p, 1 - V_{j}^p).$$  (4.38)

If an initial state $\{V_j^0\}_{0 \leq j \leq N}$ is set to be 0 or 1 for each $j$, then $V_j^p$ is determined to be either 0 or 1 in each time step. Hence, (4.38) is a cellular automaton modeling a diffusion process.
4.5.2 Ultradiscrete Lotka–Volterra equations

Now, we show the process of deriving ultradiscrete equations from nonlinear differential equations, taking the Lotka–Volterra equations (4.23) as an example.

First, we use a transformation of variables analogous to that in (4.31). Letting \( U^n_j \) be an integer and \( \varepsilon > 0 \), we transform \( U^n_j \) and \( k \) into

\[
u^n_j = e^{U^n_j/\varepsilon}, \quad k = e^{-1/\varepsilon}.
\]

Substituting these new variables into (4.22), we have

\[
\frac{e^{U^n_j + 1/\varepsilon}}{e^{U^n_j/\varepsilon}} = \frac{1 + ke^{U^n_j+1/\varepsilon}}{1 + ke^{U^n_j/\varepsilon}}.
\]

After computing the logarithm of both sides above and some calculations, we see that the \( U^n_j \)'s satisfy

\[
U^{n+1}_j = U^n_j + \varepsilon \log(1 + ke^{U^n_j+1/\varepsilon}) - \varepsilon \log(1 + ke^{U^n_j/\varepsilon})
\]

\[
= U^n_j + \varepsilon \log(1 + e^{U^n_j+1/\varepsilon}) - \varepsilon \log(1 + e^{U^n_j+1/\varepsilon}) - \varepsilon \log(1 + e^{U^n_j+1/\varepsilon}).
\]

(4.39)

It follows from Lemma 4.1 that the limit as \( \varepsilon \to 0 \) gives the following ultradiscrete Lotka–Volterra equation

\[
U^{n+1}_j = U^n_j + \max(0, U^n_{j-1} - 1) - \max(0, U^{n+1}_{j+1} - 1).
\]

(4.40)

Note that the right-hand side of (4.40) has the term at time \( n + 1 \), namely, \( U^{n+1}_{j+1} \). Therefore, the time evolution of (4.40) cannot be obtained easily even if an initial state is given, which implies that this has not become a cellular automaton yet. To obtain a cellular automaton, we need more calculations.

It is known that the bilinear differential equation (4.10) has the following explicit solution:

\[
f_j(t) = \sum_{S \subseteq \{1,2,...,N\}} \exp\left(\sum_{m \in S} \xi_m(j,t) + \sum_{l<m} a_{lm}\right),
\]

(4.41)

where

\[
\xi_m(j,t) = \delta_m j - \omega_m t + c_m, \quad \omega_m = 2 \sinh \delta_m,
\]

\[
a_{lm} = \log\left(\frac{\sinh^2 \delta_l - \delta_m}{2 \sinh^2 \delta_l + \delta_m}\right).
\]

If the parameters \( \delta_m \) and \( c_m \) are given for \( 1 \leq m \leq N \) with a natural number \( N \), then \( \omega_m, \xi_m(j,t), a_{lm} \) are fixed, and \( f_j(t) \) is determined by (4.41).

On the right-hand side of (4.41), the sum is taken over all subsets \( S \) of \( \{1,2,...,N\} \) (including the empty set). The symbol \( \sum_{m \in S} \) stands for the sum over all elements in \( S \), and \( \sum_{l<m} \) is the sum over all pairs of elements in \( S \) satisfying \( l < m \). Here, if \( S = \emptyset \), then \( \sum_{m \in S} \) is equal to 0. If \( S \) consists of only one integer, then \( \sum_{l<m} \) is defined to be 0.

Since (4.10) has the explicit solution (4.41), we see that the discrete bilinear equation (4.14) has the following solution:

\[
f^n_j = \sum_{S \subseteq \{1,2,...,N\}} \exp\left(\sum_{m \in S} \xi_m(j,n) + \sum_{l<m} a_{lm}\right),
\]

(4.42)

where

\[
\xi_m(j,n) = \delta_m j - \omega_m n + c_m, \quad \omega_m = \log\frac{1 + k(1 + e^{\delta_m})}{1 + k(1 + e^{-\delta_m})},
\]

\[
a_{lm} = \log\left(\frac{\sinh^2 \delta_l - \delta_m}{2 \sinh^2 \delta_l + \delta_m}\right).
\]

The difference between (4.41) and (4.42) lies in the replacement of \( t \) in (4.41) by \( n \) in (4.42). The definition of \( \omega_m \) is also changed.

Now, we come to the derivation of a cellular automaton from (4.40). To use the explicit solution (4.42) of (4.14), we first make an ultradiscrete equation of (4.14). Transform \( f^n_j \) and \( k \) into

\[
f^n_j = e^{f^n_j/\varepsilon}, \quad k = e^{-1/\varepsilon}.
\]

Substituting the above into (4.14) and computing the logarithm of both sides of the resulting equation, we obtain
Letting $\varepsilon \to +0$ on both sides of (4.43), we have the following ultradiscretized counterpart of equation (4.14):

$$ F_{j+1}^n + F_j^n + \varepsilon \log(1 + e^{-1/\varepsilon}) = \log(e^{F_{j+1}^n + F_j^n + 1} + e^{F_{j-1}^n + F_j^n - 1}) .$$  (4.43)

Now, recall the formula (4.15) which defines the relation between $u_j^n$ and $f_j^n$. Using (4.15) together with $u_j^n = e^{F_j/\varepsilon}$ and $f_j^n = e^{F_j/\varepsilon}$, we obtain a relation between $U_j^n$ and $F_j^n$. Indeed, since it follows from (4.15) that

$$ e^{F_j/\varepsilon} = e^{F_{j-1} - F_j} ,$$

we have the following identity after computing the logarithm of both sides:

$$ U_j^n = F_{j-1}^n + F_j^n - F_j^n + 1 .$$  (4.45)

It is clear that equation (4.44) has an explicit solution which is given by ultradiscretizing (4.42). Let $\delta_m$, $\omega_m$ and $c_m$ in (4.42) be transformed into

$$ \delta_m = \frac{K_m}{\varepsilon}, \quad \omega_m = \frac{\Omega_m}{\varepsilon}, \quad c_m = \frac{C_m}{\varepsilon} .$$

Moreover, let $\xi_m(j, n) = \Xi_m(j, n)/\varepsilon$ and $a_{lm} = A_{lm}/\varepsilon$. Then, an explicit solution of (4.44) is obtained by taking the limit of (4.42) as $\varepsilon \to +0$:

$$ F_j^n = \max_{S \subseteq \{1, 2, \ldots, N\}} \left( \sum_{m \in S} \Xi_m(j, n) + \sum_{l \in S} a_{lm} \right) ,$$  (4.46)

where

$$ \Xi_m(j, n) = K_m j - \Omega_m n + C_m ,$$

$$ \Omega_m = \max(0, K_m - 1) - \max(0, -K_m - 1) ,$$

$$ A_{lm} = |K_l - K_m| - |K_l + K_m| .$$

On the right-hand side of (4.46), $\max_{S \subseteq \{1, 2, \ldots, N\}}$ denotes the maximum over all the subsets $S$ of $\{1, 2, \ldots, N\}$. From (4.45) and (4.46), we get an explicit solution of the ultradiscrete Lotka–Volterra equation in the case $N = 1$. When $N = 1$, the quantities $F_j^n$ defined by (4.46) satisfies

$$ F_j^n = \max(0, K_1 j - \Omega_1 n + C_1) .$$

Letting $K_1 = 3$ and $C_1 = 0$ for simplicity, we see $\Omega_1 = 2$. Therefore, we have

$$ F_j^n = \max(0, 3j - 2n) .$$

It follows from (4.45) that $U_j^n$ satisfies

$$ U_j^n = \max(0, 3j - 2n - 3) + \max(0, 3j - 2n + 4)$$

$$ = \max(0, 3j - 2n) - \max(0, 3j - 2n + 1) .$$  (4.47)

Note that the right-hand side of (4.47) attains not only 0 and 1 but also other integer. If we modify (4.47) to take only 0 or 1, then it becomes a cellular automaton. We see the transformation

$$ B_j^n = F_{j-n+1}^n + F_{j-n}^{n-1} - F_{j-n}^n - F_{j-n}^n$$

leads to a cellular automaton. When $N = 1, K_1 = 3$ and $C_1 = 0$, the sequence $B_j^n$ satisfies

$$ B_j^n = \max(0, j - 3n + 3) + \max(0, j - 3n - 1)$$

$$ = \max(0, j - 3n + 3) - \max(0, j - 3n + 4) .$$  (4.48)

because of $F_j^n = \max(0, 3j - 2n)$. It can be checked that relation (4.48) defines a cellular automaton.

When $N = 2$, the sequence $B_j^n$ defined by (4.48) exhibits the time evolution shown in Figure 4.1 for appropriate constants. The rules to obtain Figure 4.1, which were explained at the beginning of Section 4, can be written in terms of the mathematical equation as follows:

$$ B_j^{n+1} = \min \left( 1 - B_j^n, \sum_{l=-\infty}^{l=\infty} (B_l^n - B_l^{n+1}) \right) .$$  (4.49)

On the right-hand side of (4.49), the term $1 - B_j^n$ shows that the cell is either empty or not at position $j$ and at time $n$. Indeed, if $B_j^n = 0$ (cell is empty), then $1 - B_j^n = 1$, while if $B_j^n = 1$ (cell is occupied), then $1 - B_j^n = 0$. Concerning the second term in the minimum function on the right-hand side of (4.49), it means...
This quantity is the amount of balls which we have at position \( j \) and at time \( n \). Hence, relation (4.49) becomes

\[
\sum_{l=-\infty}^{j-1} (B_l^n - B_l^{n+1}) = \text{(the sum of balls on the left side of the cell at position} \ j \ \text{and time} \ n) \nonumber
\]

\[
- \text{(the sum of balls on the left side of the cell with position} \ j \ \text{and time} \ n+1) \nonumber
\]

The state of cell at position \( j \) and at time \( n+1 \)

\[
= \min (\text{empty cell or not at position} \ j \ \text{and at time} \ n, \ \text{balls in hand at time} \ n) \nonumber
\]

It is clear that the right-hands side of (4.49) returns to 0 if a cell is either empty or we do not have any balls, while it returns to 1 whenever a cell is empty and we have balls, which corresponds to what is explained in Figure 4.1.

Finally, let us remark that we can introduce the ultradiscrete Lotka–Volterra equation starting from (4.49). However, there are many complicated calculations again.

5. Summary

These notes are devoted to the explanation of dynamic properties of reaction-diffusion systems modeling pattern formation, in particular, Turing patterns. Moreover, we described ideas which connect differential equations with cellular automata. More mathematical analysis of the Lengyel–Epstein model may be found in [7]. General theory about Turing patterns and their analysis are explained in [12]. Monograph [11] elaborates on the BZ reaction. For the ultradiscretization and corresponding cellular automaton, we refer the reader to [13, 14] as well as to [5, 6]. Mathematical analysis of biological models are given in [10]. Examples and remarks on numerical simulations are found in [4].

In general, mathematical models by differential equations are simplified as much as possible. For example, the BZ reaction consists of ten chemical reaction processes, but its mathematical models by kinetic systems have two or three components. If we need to know the evolution of spatial patterns for long time, reaction-diffusion equations are suitable for the purpose. On the other hand, a cellular automaton is the simplest model, which is used as models not only of pattern formation but also of other biological phenomena, crystal growth, turbulence, and so on. It is surprising that cellular automata show the complicated behaviours according to simple rules, and give us the understanding of the mechanism among a large class of phenomena. Thanks to the universal mathematical structure of cellular automata, we may be able to have a new approach for other subjects of mathematics. Indeed, complex systems as a subject of mathematics have been developed based on the studies of cellular automata.

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