Finsler geometry modeling for anisotropic diffusion in Turing patterns

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Abstract. Turing patterns are known to be described by diffusion reaction (DR) equations, and the patterns become zebra-like anisotropic if the diffusion constant is directionally dependent. However, the origin of this dependence is unclear. In this study, we report that Turing patterns can be studied with the Finsler geometry (FG) modeling technique by applying a hybrid numerical technique, which combines DR equations and the Monte Carlo (MC) technique. In the DR equations and the Hamiltonian for MC, the Finsler metric is introduced using internal degrees of freedom. We numerically show that anisotropic patterns appear according to a constraint given by some external forces applied to the internal degrees of freedom. In this FG modeling technique, direction-dependent diffusion constants are unnecessary, and these constants automatically or effectively become anisotropic. We consider that the internal degrees of freedom introduced for the Finsler metric play an essential role in the anisotropic patterns.

1. Introduction
Diffusion reaction (DR) equations introduced by A. Turing have been studied for models of random patterns such as the patterns found in zebra stripes [1]. In the equations for the abovementioned patterns, the instability of one variable in the development of time at a space point \((x, y)\) can be suppressed and stabilized by another variable, and such a stabilized pattern is propagated into the space direction by the diffusion terms. In space propagation, the patterns are deformed if diffusion constant \(D\) is directionally dependent or anisotropic, i.e., \(D_x \neq D_y\) [2]. Consequently, many anistropic patterns appear depending on this direction dependence. Therefore, anisotropic diffusion plays an important role in Turing patterns, and many studies have been conducted [3, 4, 5].

However, it is unclear why the diffusion constants become directionally dependent. For this reason, we use the Finsler geometry modeling technique. To define anisotropy in diffusion constants, we introduce dynamically changeable Finsler lengths \(v_{i,x}^{\phi,\psi}, v_{i,y}^{\phi,\psi}\) for variables \(\phi\) and \(\psi\) of the DR equations along the \(x\) and \(y\) directions at lattice site \(i\) on the regular square lattice. We numerically demonstrate that the diffusion constants effectively become anisotropic, and as a consequence, isotropic patterns become anisotropic depending on the external force along which the internal variables align.

2. Hybrid model and numerical technique
Here, we use a hybrid model, which is defined by combining the DR equations for variables \(\phi(\in \mathbb{R})\) and \(\psi(\in \mathbb{R})\) and a statistical mechanical model for internal variables \(\sigma^\phi, \sigma^\psi(\in S^1)\):
The discrete expression at site \((i,j)\) between Eqs. (3) and the Hamiltonian in Eq. (1) is correct only if \(\gamma \neq 0\), which are the well-known DR equations of FitzHugh-Nagumo. Note that the correspondence for \(D\) with a continuous Hamiltonian with diffusion constants \(\infty\) on the regular square lattice in Fig. 2(a) is of the form (a) Regular square lattice of size \((I_{max}, J_{max}) = (100, 100)\), and (b) internal variable \(\sigma_{ij}\) at the lattice site \((i,j)\), where the sites are also denoted by the numbers 0,1,2,3,4.

\[
S = S_\phi + S_\psi, \quad S_\phi = D_\phi S_{\phi,1} + S_{\phi,2}, \quad S_\psi = D_\psi S_{\psi,1} + \gamma S_{\psi,2},
\]

\[
S_{\phi,1} = \frac{1}{2} \int \sqrt{g} d^2 x \, g^{ab} \frac{\partial \phi}{\partial x^a} \frac{\partial \phi}{\partial x^b}, \quad S_{\phi,2} = - \int \sqrt{g} d^2 x \left( \frac{\phi^2}{2} - \frac{\phi^4}{4} - \frac{1}{2} \phi \psi \right),
\]

\[
S_{\psi,1} = \frac{1}{2} \int \sqrt{g} d^2 x \, g^{ab} \frac{\partial \psi}{\partial x^a} \frac{\partial \psi}{\partial x^b}, \quad S_{\psi,2} = - \int \sqrt{g} d^2 x \left( \frac{1}{2} \phi \psi - \frac{\psi^2}{2} - \beta \psi \right).
\]

The symbols \(\alpha, \beta\) and \(\gamma\) are fixed input parameters. \(g_{ab}\) is the inverse of a \(2 \times 2\) metric tensor, and \(g\) is the determinant.

Using the variational technique for \(S\) with respect to \(\delta \phi\) and \(\delta \psi\) and including the time derivative of the variables, we obtain the following partial differential equations:

\[
\frac{\partial \phi}{\partial t} = D_\phi \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \phi - \psi^3 - \psi,
\]

\[
\frac{\partial \psi}{\partial t} = D_\psi \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \gamma (\phi - \alpha \psi - \beta),
\]

for \(\gamma = -1\). For \(g_{ab} = \delta_{ab}\), the equations become

\[
\frac{\partial \phi}{\partial t} = D_\phi \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) + \phi - \psi^3 - \psi,
\]

\[
\frac{\partial \psi}{\partial t} = D_\psi \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) + \gamma (\phi - \alpha \psi - \beta),
\]

which are the well-known DR equations of FitzHugh-Nagumo. Note that the correspondence between Eqs. (3) and the Hamiltonian in Eq. (1) is correct only if \(\gamma = -1\).

The next step is to introduce Finsler lengths \(v_x^0\) and \(v_y^0\) along the \(x\) and \(y\) directions at \((x, y)\). The discrete expression at site \(i\) on the regular square lattice in Fig. 2(a) is of the form

\[
v_{i,x}^0 = |\sigma_{i,x}^0| + v_0^\phi, \quad v_{i,y}^0 = |\sigma_{i,y}^0| + v_0^\phi, \quad \text{(type C)}
\]

\[
v_{i,x}^0 = |\sigma_{i,x}^\phi| + v_0^\phi, \quad v_{i,y}^0 = |\sigma_{i,y}^\phi| + v_0^\phi, \quad \text{(type S)}
\]

where \(\sigma_{i,x(y)}^\phi\) is the \(x\) (or \(y\)) component of an internal degree of freedom \(\sigma_{i}^\phi\) at site \(i\) (Fig. 2(b)), and \(v_0^\phi\) is the cutoff, which effectively plays a role in the anisotropy strength of variable \(\phi\). The
other Finsler lengths $v^φ_i$ and $v^ψ_i$ for variable $ψ$ are defined by variable $σ^φ_i$ in exactly the same manner. Using these expressions, we introduce two different Finsler matrices, $g^φ_{ab}$ and $g^ψ_{ab}$, such that

$$g^φ_{ab} = \begin{pmatrix} \left(1/v^φ_{i,x}\right)^2 & 0 \\ 0 & \left(1/v^φ_{i,y}\right)^2 \end{pmatrix}, \quad g^ψ_{ab} = \begin{pmatrix} \left(1/v^ψ_{i,x}\right)^2 & 0 \\ 0 & \left(1/v^ψ_{i,y}\right)^2 \end{pmatrix}. \tag{5}$$

The discrete expressions for $S^φ$ and $S^ψ$ are obtained by replacing differentials $∂φ/∂x^1, ∂φ/∂x^2$ with differences $φ_i - φ_0, φ_2 - φ_0$ and integral $\int \sqrt{g} dx$ with the sum over vertices $\sum_i (v_0 v_{i0})^{-1}$.

Thus, by including several terms for the internal variable $σ$, we have the discrete Hamiltonian such that

$$S = D_φ S^φ_1 + D_ψ S^ψ_1 + γ S^φ_2 + λ_φ S^φ_0 + λ_ψ S^ψ_0 + S^φ_E + S^ψ_E,$$

$$S^φ_1 = \sum_{ij} γ^φ_{ij} (φ_j - φ_i)^2, \quad S^φ_2 = -\sum_i \frac{1}{v^φ_{i,x} v^φ_{i,y}} \left(\frac{φ_i^2}{2} - \frac{φ_i^4}{4} - φ_i ψ_i\right),$$

$$S^ψ_1 = \sum_{ij} γ^ψ_{ij} (ψ_j - ψ_i)^2, \quad S^ψ_2 = -\sum_i \frac{1}{v^ψ_{i,x} v^ψ_{i,y}} \left(ψ_i φ_i^2/2 - ψ_i^2/2 - β ψ_i\right), \tag{6}$$

$$S^φ_0 = \frac{1}{2} \sum_i \left[1 - 3 \left(σ^φ_i \cdot σ^φ_j\right)^2\right], \quad S^ψ_0 = \frac{1}{2} \sum_i \left[1 - 3 \left(σ^ψ_i \cdot σ^ψ_j\right)^2\right],$$

$$S^φ_E = -E_φ \sum_i σ^φ_i \cdot ⃗e_φ, \quad E_φ = E^φ ⃗e_φ, \quad S^ψ_E = -E_ψ \sum_i σ^ψ_i \cdot ⃗e_ψ, \quad E_ψ = E^ψ ⃗e_ψ,$$

where $ij$ in $S^φ_1$ and $S^ψ_1$ are given by

$$γ^φ_{ij} = \frac{1}{4} \left(\frac{v^φ_{i,x}}{v^φ_{j,x}} + \frac{v^φ_{i,y}}{v^φ_{j,y}}\right), \quad γ^ψ_{ij} = γ^φ_{ij}. \tag{7}$$

The Lebwohl-Lasher potential, $S^φ_0$, is assumed to be between $σ$s. The partition function is defined by $Z = \int \prod_{i=1}^N dσ^φ_i \prod_{i=1}^N dσ^ψ_i \exp(-S)$, where $\int \prod_{i=1}^N dσ^φ \prod_{i=1}^N dσ^ψ$ denotes a $2N$-dimensional multiple integration. The Hamiltonian in Eq. (6) is used only to update variables $σ^φ$ and $σ^ψ$.

The simulation procedure is as follows: The first step is to update variables $σ^φ$ and $σ^ψ$ by the canonical (or Metropolis) Monte Carlo (MC) technique. These variables are randomly updated to a new $σ'(∈ S^1)$, independent of the old $σ$, with the probability $\min[1, \exp(-δS)]$, and hence, the acceptance rate is not controllable. This first step is performed for sufficiently many MC sweeps (MCSs). The next step is to solve the DR equations in (2) with an iteration technique. These two steps are repeated. The initial configurations of $σ^φ, ψ$ are randomly generated, and hence, the total number of first iterations for the convergent configuration of the DR equations is relatively large compared to those of the second and later steps because the convergent configurations of $φ$ and $ψ$ are used as the initial configurations for the following iterations of the DR equations. We use $100 \times 100$ regular square lattices with periodic boundary conditions (2(a)), and the total number of MCSs for $σ^φ, ψ$ is $10^5$ for each step. The discrete time step $Δt$ and lattice spacing $Δx$ for the discretized DR equations corresponding to (2) are $Δt = 0.001$ and $Δx = 1$.

3. Simulation results and summary

We show snapshots of isotropic (Fig. 2(a)) and anisotropic patterns (Figs. 2(b) and (c)). The parameters in Eq. (6) are fixed to $(D^φ, D^ψ, α, β, γ) = (0.05, 5, 1, 0, 8)$ for both the DR equations.
Figure 2. Snapshots of the equilibrium configurations generated by (a) randomly distributed $\sigma^\phi$ and $\sigma^\psi$, (b),(c) $\sigma^\phi$ is random and $\sigma^\psi$ is anisotropic, where both $\nu^\phi$ and $\nu^\psi$ are Type C in (b), and both $\nu^\phi$ and $\nu^\psi$ are Type S in (c).

and MC simulation. The other parameters for the MC simulations in Eq. (6) are fixed to $(\lambda^\phi, \lambda^\psi, E^\phi, E^\psi) = (0, 0, 0, 0)$ for the isotropic pattern and $(\lambda^\phi, \lambda^\psi, E^\phi, E^\psi) = (0, 2, 0, 20)$ for the anisotropic patterns. Parameters $r_0^{\phi,\psi}$ in Eq. (4) are fixed to $r_0^{\phi,\psi} = 3$.

We study Turing patterns with a new numerical technique, which is a hybrid of MC simulations and DR equations. The Hamiltonian assumed in MC corresponds to the DR equation of FitzHugh-Nagumo, although the correspondence is not exact. The main purpose is to check whether the FG modeling technique is applicable to anisotropic diffusion, which plays a crucial role in the DR equations. From the preliminary results, we find that anisotropic patterns can be obtained by the FG modeling technique with direction-independent (or isotropic) diffusion constants $D^\phi,\psi$. This implies that the mean values of $D^{\phi,\psi} \gamma^\phi_{ij}$ in $S_1^\phi$ or $S_1^\psi$ effectively become directionally dependent.

In the FG modeling in this presentation, the directional dependence of $\gamma^\phi_{ij}$ is dynamically generated by internal degrees of freedom $\sigma^\phi,\psi (\in S^1)$, which are controlled by external force $\vec{E}^\phi,\psi$. As a consequence, two different Finsler lengths corresponding to $\sigma^\phi$ and $\sigma^\psi$ are introduced. Due to these new internal variables, the model appears slightly complex; however, it should be emphasized that these variables allow us to discuss the origin of anisotropy in the diffusion constants. This is new and in sharp contrast to the case of the original differential equation model, where the diffusion constants are input parameters and are not dynamically modified.

One more point that should be emphasized is that so-called differential equation models can be studied by Finsler geometry modeling. For more detailed information, further numerical simulations remain to be performed, and this will be a future study.

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