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IRREGULARITY OF TURING PATTERNS IN THE THOMAS MODEL WITH A UNILATERAL TERM

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Abstract

In this contribution we add a unilateral term to the Thomas model and investigate the resulting Turing patterns. We show that the unilateral term yields nonsymmetric and irregular patterns. This contrasts with the approximately symmetric and regular patterns of the classical Thomas model. In addition, the unilateral term yields Turing patterns even for smaller ratio of diffusion constants. These conclusions accord with the recent findings about the influence of the unilateral term in a model for mammalian coat patterns [3]. This indicates that the observed effects of the unilateral term are general and apply to a variety of systems.

1. Introduction

Systems of reaction-diffusion equations are widely used to model various phenomena in biology and chemistry. Spatio-temporal ecological models (e.g. predator-prey models), chemical kinetics and tumour growth can serve as examples. In addition, reaction-diffusion systems have successfully explained the spontaneous emergence of skin and coat patterns in mammals, fish, gastropods and others. One of the well-established reaction-diffusion models is the Thomas reaction kinetics model [9]. It has originally been used for modelling of chemical reactions involving oxygen and uric acid. However, Murray in [7] showed that this model can successfully model the formation of coat patterns in mammals.

The mechanism responsible for the creation of spatial patterns is known as the Turing diffusion driven instability [10]. This instability occurs if a spatially homogeneous stationary solution is stable with respect to small spatially homogeneous perturbations and unstable with respect to small spatially heterogeneous perturbations. A new stable and spatially heterogeneous steady state solution can evolve in this case and it is called a pattern. Turing instability is well known and necessary conditions for its emergence are derived, e.g. in [7], under the condition that the corresponding nonlinear terms are smooth.

The main idea of this paper is to consider the Thomas model appended by a non-smooth unilateral term. Reaction-diffusion systems with unilateral terms, mainly

in the form of variational inequalities, have been studied in [1, 4, 5] and several interesting and surprising properties have been reported. For example, there are theoretical studies showing that certain unilateral systems can produce Turing patterns for virtually arbitrary ratio of diffusion coefficients. This is surprising, because the corresponding classical reaction-diffusion system (without any unilateral term) produces Turing patterns only if this ratio is sufficiently away from one.

This motivates us to study the system of reaction-diffusion equations for the evolution of concentrations $u = u(t, x, y)$ and $v = v(t, x, y)$ of two morphogens in the following form:

$$\frac{\partial u}{\partial t} = \Delta u + \gamma(a - u - h(u, v)) \text{ in } (0, T) \times \Omega, \quad (1)$$

$$\frac{\partial v}{\partial t} = d\Delta v + \gamma(\alpha b - \alpha v - h(u, v) + \tau(v - \hat{v})^-) \text{ in } (0, T) \times \Omega \quad (2)$$

where

$$h(u, v) = \frac{\rho uv}{1 + u + Ku^2}.$$

The model parameters $a, b, d, \alpha, \gamma, \tau, K$, and ρ are constants, \hat{v} stands for the second component of the ground state, which is defined below, T denotes the final time, $\Omega \subset \mathbb{R}^2$ is a domain, and $\tau(v - \hat{v})^-$ is the unilateral term which is multiplied by γ in order to make it proportional to the size of the domain Ω in the same manner as the other nonlinear terms. Notice that the negative part is defined as $w^- = \max(0, -w)$. For $\tau = 0$, system (1)–(2) coincides with the original Thomas model. However, in this paper we mainly consider $\tau > 0$ and study the effect of the unilateral term $\tau(v - \hat{v})^-$ on the emerging patterns.

We will couple the model (1)–(2) with zero flux boundary condition

$$\frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0 \text{ on } \partial\Omega, \quad (3)$$

where n stands for the outward unit normal vector to the boundary $\partial\Omega$. The spatially homogeneous steady state solution mentioned above is known as the ground state and it is defined as a pair $\hat{u}, \hat{v} \in \mathbb{R}$, which solves the nonlinear system

$$a - \hat{u} - h(\hat{u}, \hat{v}) = 0 \quad \text{and} \quad \alpha b - \alpha \hat{v} - h(\hat{u}, \hat{v}) = 0.$$

Clearly, the constant functions $u(t, x, y) = \hat{u}$ and $v(t, x, y) = \hat{v}$ form a stationary solution to system (1)–(2) with boundary conditions (3). The component \hat{v} of the ground state is used in (2) to define the unilateral term. Notice that it is nonsmooth exactly at the point \hat{v} . The biological motivation for the nonsmooth unilateral term in (2) and its further properties are discussed in the next section.

2. Unilateral terms

A general biological motivation and existing theoretical results for reaction-diffusion systems with unilateral terms are thoroughly discussed in [3]. In this short contribution, we only offer a short overview for the sake of completeness.

System (1)–(2) for concentrations of two morphogens diffusing within a tissue is biologically plausible, because we can expect receptors in the cell membrane that detect the local concentration v of the second morphogen. The cell then reacts in such a way that if the concentration v drops below the threshold value \hat{v} , the cell will commence to produce the second morphogen. Similarly, as soon as the concentration v reaches the threshold \hat{v} the cell stops to produce it.

This mechanism is modelled in equation (2) by the unilateral term $\tau(v - \hat{v})^-$. When v is smaller than the threshold \hat{v} , the term $(v - \hat{v})^-$ becomes positive and the concentration v starts to increase with the rate $\gamma\tau|v - \hat{v}|$. In other words, the unilateral source term starts to be active. When the concentration v decreases to the level of the threshold \hat{v} , the unilateral term $\tau(v - \hat{v})^-$ vanishes and ceases to have any effect in the system.

From both the biological and mathematical point of view it is natural to set the threshold to the value \hat{v} of the ground state. Naturally, the parameter τ governs the intensity of the unilateral term.

If $\tau = 0$ then all nonlinear terms in system (1)–(2) are smooth and the standard linear analysis, see e.g. [7], can be performed to derive the necessary conditions for the Turing instability to occur. In case of system (1)–(2) this analysis restricts the diffusion coefficient d to be sufficiently large, see below. However, recent results [1, 4, 5] surprisingly revealed that this condition on d can be relaxed if certain unilateral terms or conditions are added to the system. This is an interesting feature both mathematically and biologically. Especially, in the light of the common critique of the Turing pattern formation mechanisms, that the diffusion constants of the two morphogens should be similar, because both the morphogens are presumed to be of a similar chemical nature.

The effects of the unilateral term on the resulting patterns have been studied in [3] using a model for generating pigment patterns on coats of leopards and jaguars [2, 6]. Paper [3] concludes that the unilateral term leads to nonsymmetric and irregular patterns and that the patterns appear even for ratios of diffusions violating the condition from the linear analysis. In this contribution, we investigate the Thomas model to see if we can obtain comparable results as in [3]. This would confirm that the conclusions of [3] are more general and do not apply to one specific model only.

3. Numerical results

We solve system (1)–(2) numerically using own finite element solver based on triangular meshes. The Matlab built-in adaptive time-stepping ODE solver `ode15s` is used for the time integration. We use the following set of parameters:

$$a = 150, b = 100, \alpha = 1.5, \gamma = 252, K = 0.05, \rho = 13. \quad (4)$$

We vary the diffusion coefficient d between 22.5 and 27.5 and the intensity of the unilateral source τ between 0 and 2. The domain is a square $\Omega = (-2, 2)^2$ and the computation is terminated at the final time $T = 4$ as the solution of the system

is already close to the steady state at this point. The ground state for parameter values (4) is approximately $(\hat{u}, \hat{v}) = (37.7380, 25.1588)$. The initial condition is chosen as a small random noise around this ground state. The same initial condition is used for all presented results.

Using these parameter values, we perform a numerical experiment to study the effects of the intensity of the unilateral source τ and the diffusion coefficient d on the resulting Turing patterns. Since both components u and v provide complementary results, we present plots based on v only. Figure 1 shows the resulting Turing patterns for various values of parameters τ and d .

First, we observe the qualitative change of the patterns with growing τ , see the first column in Figure 1. For $\tau = 0$ the pattern consists of close-to-circular spots with similar sizes. These spots are almost symmetrically placed. As the intensity of the unilateral term τ grows, the spots become irregular and gradually more and more elongated. The larger spots seem to be fused from several smaller ones. Starting from the value $\tau = 1$ the pattern is already substantially nonsymmetric and it is qualitatively distinct from the close to regular pattern for $\tau = 0$.

Another outcome of the performed experiment is that the unilateral term enables patterns even for d smaller than the usual linear theory [7] permits. Indeed, if $\tau = 0$ system (1)–(2) contains no unilateral term, the remaining nonlinearities are smooth, and the standard linear analysis of the Turing instability [7] yields the following critical value [8] for the diffusion coefficient d :

$$d_{\text{crit}} = \frac{\det B - b_{12}b_{21} + 2\sqrt{-b_{12}b_{21} \det B}}{b_{11}} \approx 27.027, \quad (5)$$

where

$$B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} = -\gamma \begin{bmatrix} 1 + \partial h / \partial u & -\partial h / \partial v \\ \partial h / \partial v & \alpha + \partial h / \partial v \end{bmatrix} (\hat{u}, \hat{v}) \approx \begin{bmatrix} 226.7 & -1124.5 \\ 478.7 & -1502.5 \end{bmatrix}$$

is the Jacobi matrix of system (1)–(2) evaluated at the ground state and the numerical values correspond to (4). The original Thomas model (i.e. the case $\tau = 0$) can exhibit Turing instability only if $d > d_{\text{crit}}$.

We may verify this condition in the first row of Figure 1. The second and subsequent columns of Figure 1 show that as the intensity of the unilateral source τ grows, Turing patterns emerge even for the diffusion coefficient smaller than the critical value (5). In general, this indicates that the additional unilateral term can weaken the condition on the diffusions and enables the emergence of patterns for diffusion coefficients of the two morphogens closer to each other.

4. Conclusions

This contribution evaluates the effect of the additional unilateral source term in the Thomas reaction-diffusion system. We have observed that patterns in systems with sufficiently intensive unilateral term are less regular and symmetric compared

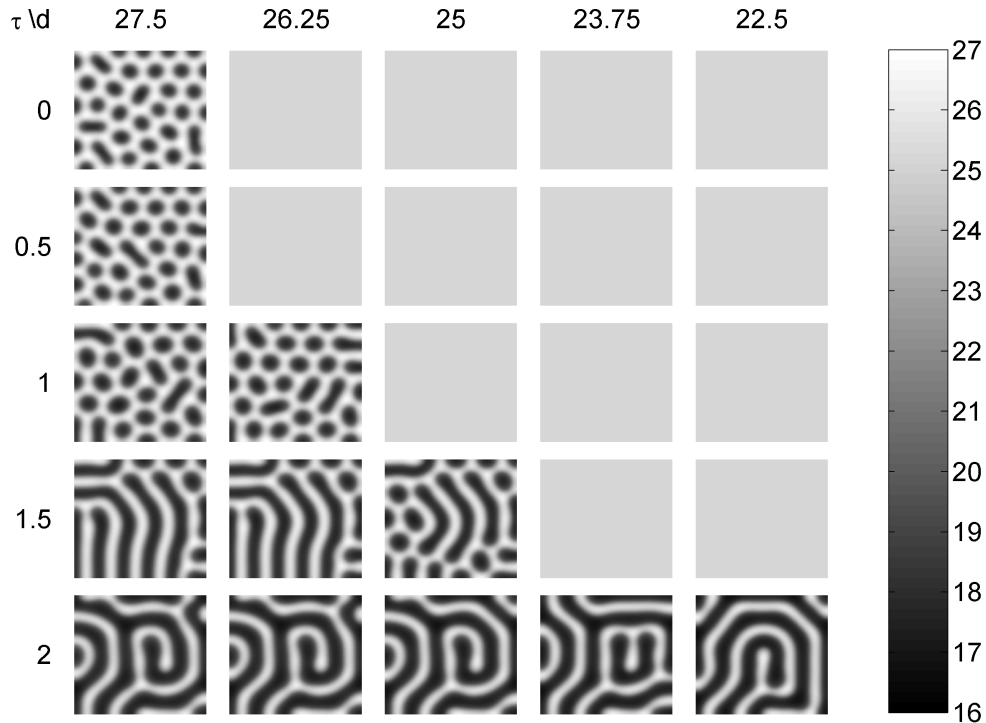


Figure 1: Patterns for various values of the intensity of the unilateral source τ and diffusion coefficient d

to patterns in systems with a weak or no unilateral term. Further, in comparison with classical systems with no unilateral regulation, the unilateral term can enable the emergence of Turing patterns even for those values of the diffusion coefficient d which prevent the Turing instability in the classical systems.

These results accord with conclusions of a more detailed study [3], where a reaction-diffusion model for coat patterns of leopard and jaguar [2, 6] is analysed. Thus, the reported effects of the unilateral source term seem to be more general and valid for more types of reaction-diffusion systems. Beside this, the observed effects verify and illustrate theoretical findings of [4], where a unilateral regulation in terms of variational inequalities is presented.

From the practical point of view, it has been suggested in [3] that the unilateral source term can explain the irregular mutant colouration observed in certain mammals, such as king cheetahs.

Reaction-diffusion systems have been studied for several decades, the corresponding literature is wide and various perspectives are already covered. However, this contribution as well as the paper [3] confirm that there are still aspects, such as the

unilateral source terms that are interesting from both theoretical and practical point of view and that deserve further investigations.

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