The theory of reaction-diffusion system on stationary domains

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December 4, 2011

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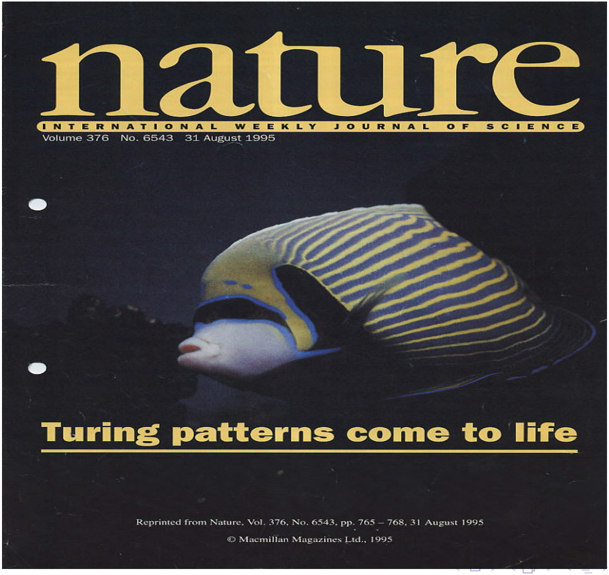
Turing patterns come to life (Asai and Kondo, 1995)



nature

INTERNATIONAL WEEKLY JOURNAL OF SCIENCE

Volume 376 No. 6543 31 August 1995

Turing patterns come to life

Reprinted from Nature, Vol. 376, No. 6543, pp. 765 – 768, 31 August 1995

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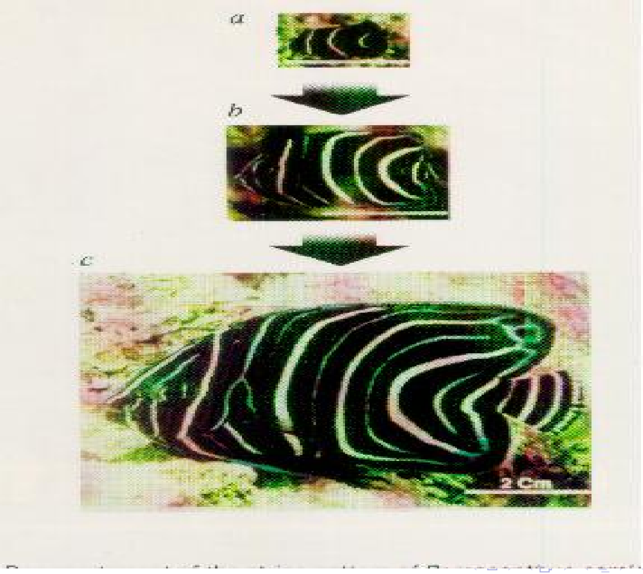
Pomacanthus zebra fish (Asai and Kondo, 1995)

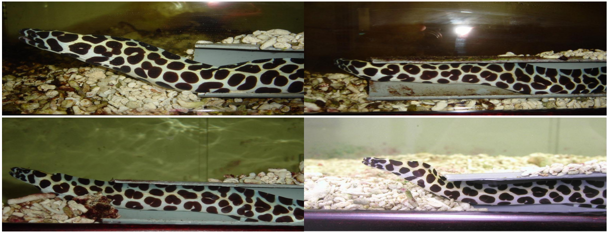


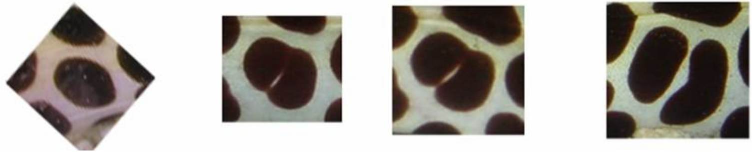
Juvenile Pomacanthus

Adult Pomacanthus

Transient/Evolution of Patterns

Leopard eel patterns (Kondo, 2007)





Global patterning on butterfly wings

meriones

Homozygous
forms of
Papilio dardanus

antinorii

poultoni

ochracea

hippocoonides

trophonius

dionysos

leighi

lamborni

planemoides

Basic Notation: Spaces and norms

Here we introduce some basic notation that will be used throughout this lecture. We begin by introducing the following functional spaces and norms.

Let $\Omega_t \subset \mathcal{R}^2$ be a simply connected bounded continuously evolving domain at time $t \in I = [0, T_f]$, $T_f > 0$ and $\partial\Omega_t$ be its continuously deforming boundary. Taking $1 \leq p < \infty$, we define

$$L^p(\Omega_t) = \left\{ v(\mathbf{x}, t) : \int_{\Omega_t} |v(\mathbf{x}, t)|^p \, d\Omega_t < \infty \text{ for } \mathbf{x} \in \Omega_t, \; t \in I \right\}$$

and its corresponding norm

$$\|v(\mathbf{x}, t)\|_{L^p(\Omega_t)} = \left(\int_{\Omega_t} |v(\mathbf{x}, t)|^p \, d\Omega_t \right)^{\frac{1}{p}}.$$

The set $L^p(\Omega_t)$ is a Banach space.

Basic Notation: Spaces and norms

We define the following Hilbert space on $\Omega_t, \; t \in I$.

$$H^1(\Omega_t) = \Big\{ v(\mathbf{x}, t) \in L^1(\Omega_t), \, D^{\boldsymbol{\alpha}} v \in L_1(\Omega_t), \; |\boldsymbol{\alpha}| \leq 1 \Big\},$$

for every $t \in I$, where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2)$, $|\boldsymbol{\alpha}| = \alpha_1 + \alpha_2$ and $D^{\boldsymbol{\alpha}}$ represents the distributional derivative at every time $t \in I$,

$$D^{\boldsymbol{\alpha}} v = \frac{\partial^{|\boldsymbol{\alpha}|} v}{\partial^{\boldsymbol{\alpha}_1} x \, \partial^{\boldsymbol{\alpha}_2} y}.$$

Reynolds transport theorem

This theorem will be useful in the derivation of the reaction-diffusion systems on evolving domains and also for the numerical method. The theorem states:

Theorem

(Reynolds transport theorem) Let $g(\boldsymbol{x}, t)$ *be a scalar function defined on* Ω_t *and* $\boldsymbol{\beta}$ *be a flow velocity field then*

$$\frac{d}{dt}\int_{\Omega_t} g \, d\Omega_t = \int_{\Omega_t} \left(\partial^{\bullet} g + g\nabla \cdot \boldsymbol{\beta}\right) \, d\Omega_t \tag{1}$$

where

$$\partial^{\bullet} g := g_t + \boldsymbol{\beta} \cdot \nabla_{\Gamma_t} g$$

defines the material derivative following the flow.

Proof.

See Madzvamuse, 2000, Acheson, 1990; and Marsden and Chorin, 1993. ☐

Derivation of RDEs on evolving domains

Following Madzvamuse (2000), let $\boldsymbol{u} = \left(u\left(\boldsymbol{x}(t), t\right), v\left(\boldsymbol{x}(t), t\right)\right)^T$ be a vector of two chemical concentrations at position $\boldsymbol{x} = (x(t), y(t), z(t)) \in \Omega_t \subset \mathbb{R}^m$. For each concentration we have a mass conservation law which balances the rate of change of the concentration in an evolving material region of the domain with the outward flux and a net reactive production rate of the chemical within the domain. Let $\mathcal{R}_t$ be an arbitrary material portion of Ω_t where each point moves with the material velocity. Let us consider the u concentration for illustrative purposes. According to the mass balance conservation law,

$$\frac{d}{dt}\int_{\mathcal{R}_t} u(\boldsymbol{x}, t) = -\int_{\partial\mathcal{R}_t} \boldsymbol{F}\cdot d\boldsymbol{S} + \int_{\mathcal{R}_t} f_1(u, v) \tag{2}$$

where $\boldsymbol{F}$ is the flux through the boundary of $\mathcal{R}_t$ and $f_1(u, v)$ represents the net production within the domain.

Derivation of RDEs on evolving domains

Using the Transport and the Divergence Theorems leads to the equation

$$\int_{\mathcal{R}_t} \left(\partial^{\bullet} u + u\left(\nabla \cdot \boldsymbol{\beta}\right) + \nabla \cdot \boldsymbol{F} - f_1(u,v)\right) = 0. \tag{3}$$

Furthermore, applying the definition of the material derivative results in the following conservative equation

$$\int_{\mathcal{R}_t} \left(u_t + \boldsymbol{\beta} \cdot \nabla u + u\left(\nabla \cdot \boldsymbol{\beta}\right) + \nabla \cdot \boldsymbol{F} - f_1(u,v)\right) = 0. \tag{4}$$

Since $\mathcal{R}_t$ is arbitrary for all time t, we conclude that

$$u_t + \nabla \cdot (\boldsymbol{\beta} u) + \nabla \cdot \boldsymbol{F} - f_1(u,v) = 0. \tag{5}$$

Derivation of RDEs on evolving domains

For the constitutive law relating the flux to the concentrations, assuming no cross-diffusion between the chemical species, we set D_u to be a constant diffusion coefficient corresponding to the chemical concentration u. The standard assumption is that the chemical flux is proportional to the concentration gradient (this is known as Fick's law)

$$\boldsymbol{F} = -D_u \nabla u$$

we obtain the reaction-diffusion equation on an arbitrary evolving domain

$$u_t + \nabla \cdot (\beta u) = D_u \nabla^2 u + f_1(u, v), \quad \text{in } \Omega_t. \tag{6}$$

Similarly for the v chemical concentration we have

$$v_t + \nabla \cdot (\beta v) = D_v \nabla^2 v + f_2(u, v), \quad \text{in } \Omega_t. \tag{7}$$

Contributions from domain evolution

Remark

The terms $\nabla \cdot (\beta u)$ *and* $\nabla \cdot (\beta v)$ *represent the dilution and convective properties of the chemical species due to domain evolution. In the absence of domain growth, these terms vanish, resulting in the standard reaction-diffusion system on fixed domains (Murray, 2003).*

Boundary conditions

- Self-organisation:
  - Homogeneous Neumann boundary conditions

$$(\boldsymbol{n} \cdot \nabla u) = (\boldsymbol{n} \cdot \nabla v) = 0, \quad x \in \partial\Omega_t \; t \geq 0$$

  - Zero-flux boundary conditions
- Dirichlet boundary conditions

$$u(x,t) = c_1, \; v(x,t) = c_2$$

- Periodic boundary conditions (circles etc)

Initial conditions

Initial conditions are prescribed as follows:

$$u(x,0) = u_0(x),\ v(x,0) = v_0(x),\ x \in \Omega_0,\ t = 0,$$

where $u_0(x)$ and $v_0(x)$ are positive bounded functions.

Shnakenberg reaction-kinetics

These are derived from a series of hypothetical tri–molecular autocatalytic reactions proposed by Schnakenberg (1979):

$$X \underset{k_1}{\overset{k_2}{\rightleftharpoons}} A, \quad B \xrightarrow{k_4} Y, \quad 2X + Y \xrightarrow{k_3} 3X.$$

Denoting

$$u(t) = [X], \quad v(t) = [Y], \quad a_1 = [A], \quad \text{and} \quad b_1 = [B]$$

then by the Law of Mass Action, which states that the rate of reaction is directly proportional to the product of the active concentrations of the reactants,

$$\begin{aligned} f(u,v) &= k_1\, a_1 - k_2\, u + k_3\, u^2\, v, \\ g(u,v) &= k_4\, b_1 - k_3\, u^2 v. \end{aligned}$$

Non-dimensionalisation

Define

$$\hat{u} = u^{*}u(x,t),\ \hat{v} = v^{*}v(x,t),\ \hat{\boldsymbol{\beta}} = \beta^{*}\boldsymbol{\beta}(x,t),\ \hat{x} = \frac{x}{L_x},\ \tau = t^{*}t$$

and substituting into (6) and (7) we have

$$\begin{aligned}\hat{u}_{\tau} &= \frac{u^{*}}{t^{*}}\Big[-\nabla\cdot(\boldsymbol{\beta}\,u) + f(u,v) + D_u\,\nabla^2 u\Big]\\ \hat{v}_{\tau} &= \frac{v^{*}}{t^{*}}\Big[-\nabla\cdot(\boldsymbol{\beta}\,v) + g(u,v) + D_v\,\nabla^2 v\Big]\end{aligned}$$

Non-dimensionalisation

$$\hat{u}_\tau = \frac{u^*}{t^*}\Big[-\nabla\cdot(\boldsymbol{\beta}\, u) + k_1\, a_1 - k_2\, u + k_3\, u^2\, v + D_u\, \nabla^2 u\Big]$$
$$\hat{v}_\tau = \frac{v^*}{t^*}\Big[-\nabla\cdot(\boldsymbol{\beta}\, v) + k_4\, b_1 - k_3\, u^2 v + D_v\, \nabla^2 v\Big]$$

which reduce to

$$\hat{u}_\tau = -\frac{\nabla\cdot(\beta^*\beta\, u^* u)}{\beta^* t^*} + \frac{k_1\, a_1 u^*}{t^*} - \frac{k_2\, u^* u}{t^*} + \frac{k_3\, {u^*}^2 u^2 v^* v}{t^* u^* v^*} + \frac{D_u}{t^* L_x^2}\nabla^2(u^* u)$$
$$\hat{v}_\tau = -\frac{\nabla\cdot(\beta^*\beta\, v^* v)}{\beta^* t^*} + \frac{k_4\, b_1 v^*}{t^*} - \frac{k_3\, {u^*}^2 u^2 v^* v}{t^* {u^*}^2} + \frac{D_v}{t^* L_x^2}\nabla^2(v^* v)$$

Non-dimensionalisation

Non-dimensionalisation yields

$$\begin{aligned} \frac{\partial u}{\partial t} + \nabla \cdot (\beta u) &= \gamma\,(a - u + u^2\,v) + \nabla^2 u, \\ \frac{\partial v}{\partial t} + \nabla \cdot (\beta v) &= \gamma\,(b - u^2\,v) + d\,\nabla^2 v, \end{aligned}$$

where

$$t^* = \frac{L_x^2}{D_u},\; a = \frac{k_1\,a_1}{k_2}\sqrt{\frac{k_3}{k_2}},\; b = \frac{k_4\,b_1}{k_2}\sqrt{\frac{k_3}{k_2}},\; d = \frac{D_u}{D_v}\;\gamma = \frac{k_2\,L_x^2}{D_u},$$

$$\beta^* = \frac{D_u}{L_x^2},\; u^* = \sqrt{\frac{k_3}{k_2}} \quad \text{and} \quad v^* = \sqrt{\frac{k_4}{k_2}}.$$

Non-dimensionalised RDS on evolving domains

$$\frac{\partial u}{\partial t} + \nabla \cdot (\boldsymbol{\beta} u) = \gamma\,(a - u + u^2\,v) + \nabla^2 u,$$
$$\frac{\partial v}{\partial t} + \nabla \cdot (\boldsymbol{\beta} v) = \gamma\,(b - u^2\,v) + d\,\nabla^2 v, \quad t \in \Omega_t$$

Homogeneous Neumann boundary conditions

$$\Big[\boldsymbol{\mu} \cdot \nabla u\Big](\boldsymbol{x}, t) = \Big[\boldsymbol{\mu} \cdot \nabla v\Big](\boldsymbol{x}, t) = 0, \quad t \in \partial\Omega_t.$$

Initial conditions

$$u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}), \quad \text{and} \quad v(\boldsymbol{x}, 0) = v_0(\boldsymbol{x})$$

where $u_0(\boldsymbol{x})$ and $v_0(\boldsymbol{x})$ are non-negative bounded functions.

Non-dimensionalised RDS on stationary domains

$$\begin{aligned}\frac{\partial u}{\partial t} &= \gamma\,(a - u + u^2\,v) + \nabla^2 u,\\ \frac{\partial v}{\partial t} &= \gamma\,(b - u^2\,v) + d\,\nabla^2 v, \quad t \in \Omega\end{aligned}$$

Homogeneous Neumann boundary conditions

$$\Big[\boldsymbol{\mu}\cdot\nabla u\Big](\boldsymbol{x},t) = \Big[\boldsymbol{\mu}\cdot\nabla v\Big](\boldsymbol{x},t) = 0, \quad t \in \partial\Omega.$$

Initial conditions

$$u(\boldsymbol{x},0) = u_0(\boldsymbol{x}), \quad \text{and} \quad v(\boldsymbol{x},0) = v_0(\boldsymbol{x})$$

where $u_0(\boldsymbol{x})$ and $v_0(\boldsymbol{x})$ are non-negative bounded functions.

Equilibrium points

Definition

A uniform steady state is a fixed point $(u,v) = (u_s, v_s)$ such that u_s and v_s are constants in time and space, satisfying

$$\begin{aligned} f(u,v) &= 0, \\ g(u,v) &= 0. \end{aligned}$$

Definition

Diffusion–driven instability (or Turing instability) occurs when a uniform steady state, linearly stable in the absence of diffusion, goes unstable when diffusion is present.

Uniform steady states

Solving

$$
\begin{aligned}
f(u,v) = 0 &\iff a - u + u^2 v = 0 \\
g(u,v) = 0 &\iff b - u^2 v
\end{aligned}
$$

Adding the two equations results in

$$u = a + b$$

From

$$g(u,v) = 0 \iff b - u^2 v \iff v = \frac{b}{u^2} = \frac{b}{(a+b)^2}.$$

Therefore the uniform steady state is defined by

$$(u_s, v_s) = \left(a + b, \frac{b}{(a+b)^2} \right).$$

Linear stability in the absence of diffusion

In the absence of spatial variations, u and v satisfy

$$\frac{\partial u}{\partial t} = \gamma f(u,v) \quad \text{and} \quad \frac{\partial v}{\partial t} = \gamma\, g(u,v). \tag{8}$$

Define $|\xi| \ll 1$ and $|\eta| \ll 1$ such that $(u,v) = (u_s + \xi, v_s + \eta)$ where (u_s, v_s) is a homogeneous steady state, i.e. $f(u_s,v_s) = g(u_s,v_s) = 0$. Let $\boldsymbol{w} = (\xi,\eta)^T$, then linearising (8) about the steady state (u_s,v_s) gives

$$\begin{pmatrix} \frac{\partial u}{\partial t} \\ \frac{\partial v}{\partial t} \end{pmatrix} = \begin{pmatrix} \frac{\partial \xi}{\partial t} \\ \frac{\partial \eta}{\partial t} \end{pmatrix} = \gamma \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix} \tag{9}$$

where second order and higher order terms of ξ and η have been ignored.

Linear stability in the absence of diffusion

Taking

$$\boldsymbol{w} = e^{\lambda t}\boldsymbol{w}_0$$

it follows that

$$\lambda e^{\lambda t}\boldsymbol{w}_0 = \gamma \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} e^{\lambda t}\boldsymbol{w}_0. \tag{10}$$

Dividing by $e^{\lambda t} > 0$ results in

$$\left[\lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \gamma \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}\right] \boldsymbol{w}_0. \tag{11}$$

Since $\boldsymbol{w} \neq \boldsymbol{0}$ then

$$\left| \begin{pmatrix} \lambda - \gamma f_u & \gamma f_v \\ \gamma g_u & \lambda - \gamma g_v \end{pmatrix} \right| = \boldsymbol{0}. \tag{12}$$

Linear stability in the absence of diffusion

Computing the determinant we have

$$\lambda^2 - \gamma(f_u + g_v)\lambda + \gamma^2(f_u\, g_v - f_v\, g_u) = 0$$

which solves to give

$$\lambda_\pm = \frac{\gamma(f_u + g_v) \pm \sqrt{\gamma^2(f_u + g_v)^2 - 4\gamma^2(f_u\, g_v - f_v\, g_u)}}{2}.$$

Therefore

$$Re(\lambda) < 0$$

if and only if

$$\text{Trace } = f_u + g_v < 0, \tag{13}$$

$$\text{Determinant } = f_u\, g_v - f_v\, g_u > 0, \tag{14}$$

which implies the stability of the homogeneous steady state.

Linear instability in the presence of diffusion

Linearising

$$\frac{\partial u}{\partial t} = \gamma f(u,v) + \nabla^2 u, \tag{15}$$

$$\frac{\partial v}{\partial t} = \gamma\, g(u,v) + d\,\nabla^2 v, \tag{16}$$

about the steady state (u_s, v_s) in the presence of spatial variations we have

$$\frac{\partial \boldsymbol{w}}{\partial t} = \gamma\, \boldsymbol{J_F}\, \boldsymbol{w} + \boldsymbol{D}\,\nabla^2 \boldsymbol{w} \tag{17}$$

where $\boldsymbol{J_F} = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}$ and $\boldsymbol{D} = \text{diag}\{1, d\}$. The corresponding boundary condition is given by $(\boldsymbol{\mu}.\nabla)\,\boldsymbol{w} = 0$. Equation (17) is now a linear parabolic differential equation which can be solved by separation of variables to yield

$$\boldsymbol{w}(\boldsymbol{x},t) = \sum_k \boldsymbol{c}_k e^{\lambda t} \boldsymbol{w}_k(\boldsymbol{x}). \tag{18}$$

Linear instability in the presence of diffusion

For each k (the eigenvalue which is the wave number of the corresponding component of the spatial pattern), $\boldsymbol{c}_k$ represents the vector of Fourier coefficients and $\boldsymbol{w}_k$ is the eigenfunction of the Laplacian i.e. it satisfies

$$\nabla^2 \boldsymbol{w}_k + k^2 \boldsymbol{w}_k = 0 \tag{19}$$

with zero flux boundary conditions

$$(\boldsymbol{\mu}.\nabla)\boldsymbol{w}_k = 0. \tag{20}$$

Substituting (18)–(19) into (17) we obtain for each k, the eigenvalue problem

$$\left(\lambda \boldsymbol{I} - \gamma \boldsymbol{J_F} + \boldsymbol{D}\, k^2\right) \boldsymbol{c}_k = \boldsymbol{0}, \tag{21}$$

where $\boldsymbol{I}$ is the unit tensor. As we require non–trivial solutions for $\boldsymbol{c}_k$, the following condition must hold:

$$\left|\lambda \boldsymbol{I} - \gamma \boldsymbol{J_F} + \boldsymbol{D}\, k^2\right| = 0. \tag{22}$$

Linear instability in the presence of diffusion

It follows that $\lambda = \lambda(k^2)$ satisfies the dispersion relation

$$\lambda^2 + b(k^2)\,\lambda + c(k^2) = 0 \tag{23}$$

where

$$b(k^2) = k^2\,(1+d) - \gamma\,(f_u + g_v), \tag{24}$$
$$c(k^2) = d\,k^4 - \gamma\,(d\,f_u + g_v)\,k^2 + \gamma^2\,(f_u\,g_v - f_v\,g_u). \tag{25}$$

For diffusion–driven instability to occur one of the roots of (23) must have $\mathrm{Re}\lambda(k^2) > 0$ for some $k^2 > 0$. The condition (13) implies that $b(k^2) > 0$ for all $k^2 > 0$. Therefore $\mathrm{Re}\lambda(k^2) > 0$ only when $c(k^2) < 0$ for some $k^2 > 0$. The equation for $c(k^2)$ is quadratic in terms of k^2, so it is easy to show that $c(k^2) < 0$ (for some $k^2 > 0$) if and only if

$$d\,f_u + g_v > 0. \tag{26}$$

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Linear instability in the presence of diffusion

Solving $c(k^2) = 0$ results in

$$k_{\pm}^2 = \frac{\gamma\,(d f_u + g_v) \pm \sqrt{\gamma^2 (d f_u + g_v)^2 - 4d\gamma^2\,(f_u\, g_v - f_v\, g_u)}}{2d}.$$

For $\mathrm{Re}\lambda(k^2) > 0$ for some $k^2 > 0$ implies

$$\frac{(d f_u + g_v)^2}{4\,d} > f_u\, g_v - f_v\, g_u. \tag{27}$$

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Necessary conditions for diffusion-driven instability

Theorem

The necessary conditions for diffusion-driven instability on fixed domains are given by

$$f_u + g_v < 0, \tag{28}$$

$$f_u g_v - f_v g_u > 0, \tag{29}$$

$$d f_u + g_v > 0, \tag{30}$$

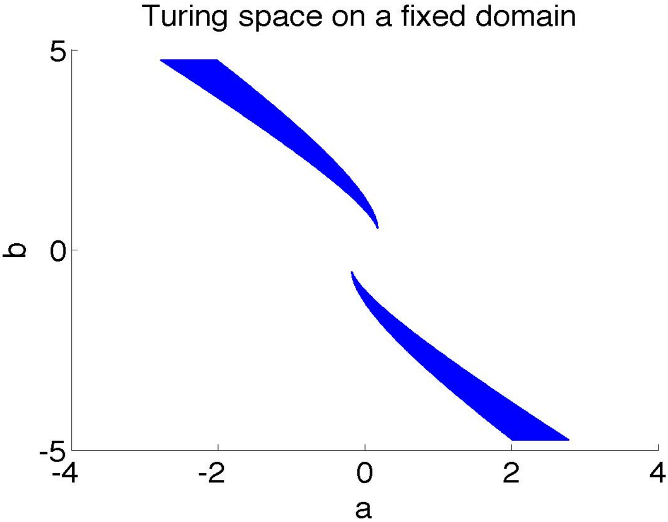
$$(d f_u + g_v)^2 - 4 d (f_u g_v - f_v g_u) > 0. \tag{31}$$

The inequalities (28)–(31) *define a domain in parameter space, known as the Turing space, wherein the uniform steady state* (u_s, v_s) *is linearly unstable.*

Proof.

See derivation above. ☐

Turing parameter space



Sufficient conditions diffusion-driven instability

- The condition $f_u + g_v < 0$ implies that $d \neq 1$ and that f_u and g_v must have opposite signs. Without loss of generality we take $f_u > 0$, so that the condition $d\, f_u + g_v > 0$ requires that d must be greater than unity.
- It is worth noting that $\min\left(c(k^2)\right) = 0$ if and only if

$$(d\, f_u + g_v)^2 = 4\, d\, (f_u\, g_v - f_v\, g_u) \tag{32}$$

which is a quadratic function in terms of d. Therefore, for fixed kinetic parameters, there exists a critical diffusion ratio d_c which is an appropriate root of the quadratic equation (32) consistent with conditions (28) and (30) above which diffusion driven instability can occur.

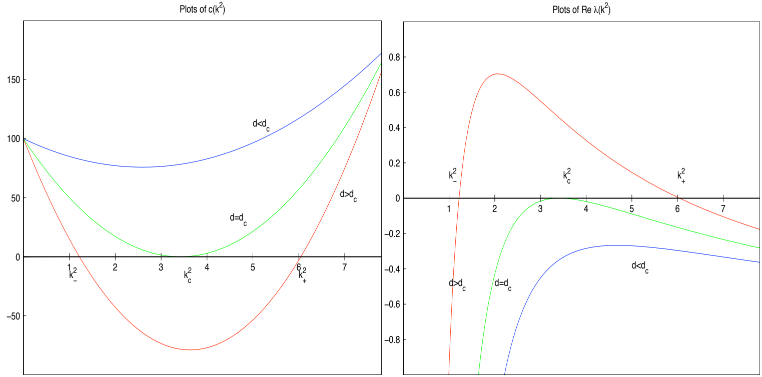
Sufficient conditions diffusion-driven instability

- Corresponding to this value of d, there is a critical wavenumber k_c, given by

$$k_c^2 = \gamma \, \frac{d_c f_u + g_v}{2\, d_c} = \gamma \sqrt{\frac{f_u\, g_v - f_v\, g_u}{d_c}}. \tag{33}$$

- The uniform steady state loses linear stability when d is greater than the critical diffusion ratio $d = d_c$, which implies that d_c is a bifurcation point.

Dispersion relation



Excitable wavenumbers

From the figure above it can be seen that there exists a range $k_-^2 < k^2 < k_+^2$ where $c(k^2) < 0$ and $\mathrm{Re}(\lambda(k^2)) > 0$ with

$$\boldsymbol{w}(\boldsymbol{x}, t) = \sum_k \boldsymbol{c}_k \, e^{[\lambda(k^2)\, t]} \boldsymbol{w}_k(\boldsymbol{x}), \qquad t \to \infty. \tag{34}$$

The values $k_\pm^2$ are the roots of the equation $c(k^2) = 0$ and are explicitly given by

$$k_\pm^2 = \gamma \, \frac{(d\, f_u + g_v) \pm \sqrt{(d\, f_u + g_v)^2 - 4\, d\, (f_u\, g_v - f_v\, g_u)}}{2\, d}. \tag{35}$$

Implications of Turing diffusion-driven instability conditions

The condition (28) implies that at least one of the two terms f_u or g_v is negative. If $g_v < 0$, for example, then the chemical concentration v inhibits its own rate of formation. It also follows that from condition (30) $f_u > 0$, that is, the chemical concentration u activates its own production. Condition (29) then implies that $f_v \, g_u < 0$. Hence there are two cases:

- $f_v < 0$ and $g_u > 0$: the reaction–diffusion system is called an activator–inhibitor system and
- $f_v > 0$ and $g_u < 0$: the system is called a positive feedback system.

Implications of Turing diffusion-driven instability conditions

The diffusive–driven instability conditions (28)–(31) imply that when $d = d_c$, the onset of instability, $\lambda(k^2)$ is purely real, so the instability is stationary, that is, oscillations occur in space but not in time. If $d < d_c$, diffusive instability does not occur. In this scenario it follows from (28) and (30) that $d > 1$. Physically this means that the inhibitor diffuses much faster than the activator, that is the range of inhibition is larger than the range of activation: *short–range activation, long–range inhibition* is a classical mechanism for self–organised patterning (Gierer and Meinhardt, 1972; Meinhardt, 1982; Edelstein–Keshet, 1988). Near a simple primary bifurcation point, the solution is well–approximated by linear analysis. However, as one moves away from the bifurcation point, the nonlinear terms can greatly complicate the solution behaviour (see Fife, 1979, for review).

Eigenfunctions in one dimension

The solution to equation (19) with boundary conditions (20) on the one–dimensional domain $[0, L_x]$ is given by

$$\boldsymbol{w}_n(x) = \cos(\frac{n\,\pi}{L_x}\,x), \quad n = \ 1,\ 2, \cdots\ . \tag{36}$$

Here the admissible wavenumbers have the form $k_n = \frac{n\pi}{L_x}$. The general solution is given by

$$\boldsymbol{w}(x,t) = \sum_n \boldsymbol{c}_n\ \exp[\lambda\left(\frac{n^2\,\pi^2}{L_x^2}\right)\ t]\cos\left(\frac{n\,\pi}{L_x}\,x\right). \tag{37}$$

Eigenfunctions of a rectangle

Consider the rectangle defined by

$$R = \{(x,y) \in \mathbb{R}^2 \,:\, 0 < x < p, \quad 0 < y < q\}.$$

The eigenfunctions in this case are of the form

$$\boldsymbol{w}_{p,q} = \cos\left(\frac{m\,\pi\,x}{p}\right)\cos\left(\frac{n\,\pi\,y}{q}\right), \quad m,n = 0,1,2,\cdots \tag{38}$$

with eigenvalues

$$k^2 = k^2_{m,n} = \pi^2\left(\frac{m^2}{p^2} + \frac{n^2}{q^2}\right).$$

Eigenfunctions of a rectangle

We expect that as $t \to \infty$, the solution of the linearised system will be of the form

$$\boldsymbol{w}(x, y, t) = \sum_{m,n \in G} \boldsymbol{C}_{m,n} \exp[\lambda(k_{m,n}^2)\, t] \cos\left(\frac{m\,\pi x}{p}\right) \cos\left(\frac{n\,\pi\, y}{q}\right) \tag{39}$$

where

$$G = \{(m, n) \in \mathbb{Z}^2 : \gamma\, L = k_-^2 < k_{m,n}^2 = \pi^2 \left(\frac{m^2}{p^2} + \frac{n^2}{q^2}\right) < k_+^2 = \gamma\, R\} \tag{40}$$

is the set of all excitable modes $(m,\ n)$ (Murray, 1993). Here

$$L = \frac{(d\, f_u + g_v) - \sqrt{(d\, f_u + g_v)^2 - 4\, d\, (f_u\, g_v - f_v\, g_u)}}{2\, d} \tag{41}$$

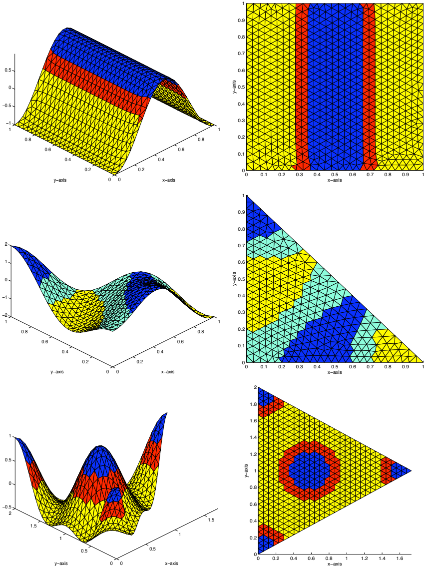
and

$$R = \frac{(d\, f_u + g_v) + \sqrt{(d\, f_u + g_v)^2 - 4\, d\, (f_u\, g_v - f_v\, g_u)}}{2\, d}. \tag{42}$$

Eigenfunctions of a unit square

Consider the eigenfunction $\cos(2\pi x)$ on the domain $[0,1]\times[0,1]$. This is not the only eigenfunction with the wave number satisfying $k^2 = 4\pi^2$ on the unit square, since $\cos(2\pi y)$ also satisfies this equation. The occurrence of more than one eigenfunction with the same wavenumber is known as degeneracy. Another example is on the domain $[0,4]\times[0,1]$, where $p = 4$ and $q = 1$, we have $k^2_{4,0} = \pi^2 = k^2_{0,1}$. Here linear stability predicts multiple solutions but does not predict the stability of the evolving solutions nor which solution is selected. In many cases the initial conditions determine the patterns selected (Murray, 1993). Hence pattern formation on fixed domains is very sensitive to initial conditions. It can be shown that the problem of sensitivity to small amplitude initial perturbations about the uniform steady state is greatly decreased on a growing domain.

Eigenfunctions on regular fixed domains



Eigenfunctions on a right–angled isosceles triangle

The eigenfunctions are given by

$$\begin{cases} \boldsymbol{w}_{m,n}(x,y) = \cos\left(\frac{\pi}{a}(m+n)x\right)\cos\left(\frac{\pi}{a}ny\right) + \cos\left(\frac{\pi}{a}(m+n)y\right)\cos\left(\frac{\pi}{a}nx\right), \\ \text{if } m \text{ is even,} \\ \boldsymbol{w}_{m,n}(x,y) = \cos\left(\frac{\pi}{a}(m+n)x\right)\cos\left(\frac{\pi}{a}ny\right) - \cos\left(\frac{\pi}{a}(m+n)y\right)\cos\left(\frac{\pi}{a}nx\right), \\ \text{if } m \text{ is odd,} \end{cases}$$

with

$$k^2 = k_{m,n}^2 = \frac{\pi^2}{a^2}[(m+n)^2 + n^2] = \frac{\pi^2}{a^2}(m^2 + 2mn + 2n^2). \tag{43}$$

Hence linear solutions are given by

$$\boldsymbol{w}(x,y,t) \approx \sum_{m,n} \boldsymbol{C}_{m,n} \exp[\lambda(k_{m,n}^2)t]\boldsymbol{w}_{m,n}(x,y) \tag{44}$$

$\boldsymbol{w}(x,y)$ takes either form depending on whether m is even or odd and the sum is over all modes with $\lambda(k_{m,n}^2) > 0$.

Eigenfunctions on equilateral triangles

Lamé (1852) and Pinsky (1980) considered an equilateral triangle of the form

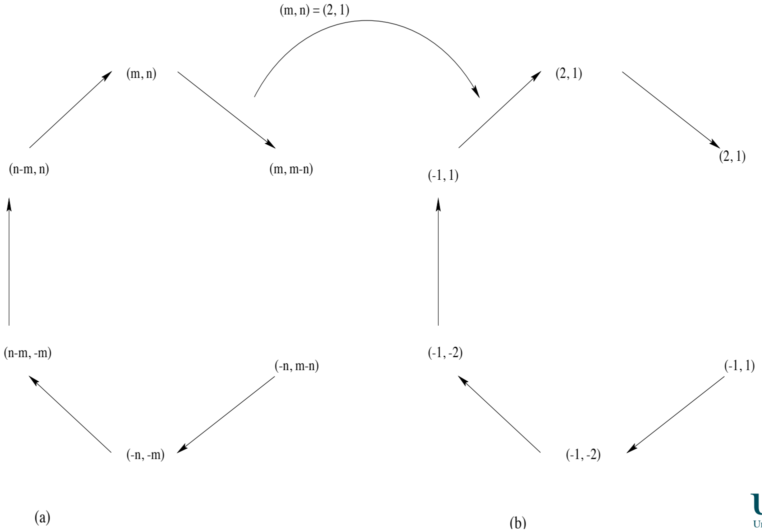
$$\triangle = \{(x,y) \in \mathbb{R}^2 : \quad 0 < y < x\sqrt{3} \quad \text{and} \quad y < (1-x)\sqrt{3}\}. \tag{45}$$

The eigenfunctions on this particular domain are given by

$$\boldsymbol{w}_{m,n}(x,y) = \sum_{(m,n)} \pm \exp[(\frac{2\pi i}{3})\left(n\,x + \frac{2\,m-n}{\sqrt{3}}\,y\right)] \tag{46}$$

where (m,n) are ordered pairs of integers a certain summation rules shown on next page.

Summation rules



Eigenfunctions on equilateral triangles

The corresponding eigenvalues on this triangle with homogeneous Neumann boundary conditions are given by

$$k^2 = k_{m,n}^2 = \frac{16\,\pi^2}{27}(m^2 + n^2 - m\,n), \qquad m, n = 0, 1, 2, \cdots \tag{47}$$

where $m + n$ is multiple of 3 (Pinsky, 1980).
In biological applications, $\boldsymbol{w}_{m,n}$ must be real, therefore we take the real part of (46), namely

$$\boldsymbol{w}(x, y, t) = \sum_{(m,n)} \pm \cos\left(\frac{2\,\pi}{3}(n\,x + \frac{2\,m - n}{\sqrt{3}}\,y)\right). \tag{48}$$

Calculation of the homogeneous steady states

The homogeneous steady state for the Schnakenberg model satisfies

$$f(u, v) = a - u + u^2 v, = 0, \tag{49}$$

$$g(u, v) = b - u^2 v = 0. \tag{50}$$

This can be calculated explicitly and is given by $(u_s, v_s) = \left(a + b, \frac{b}{(a+b)^2}\right)$. If we fix the values $a = 0.1$, $b = 0.9$ we have the steady state $(1.0, 0.9)$. The corresponding entries in the Jacobian matrix for the Schnakenberg reaction kinetics are given by

$$\begin{aligned} f_u &= -1 + 2\,u\,v, \\ f_v &= u^2, \\ g_u &= -2\,u\,v, \\ g_v &= -u^2. \end{aligned}$$

Selection of parameter values in one dimension

For simplicity let $L_x = 1$ in (36), that is, we consider a unit interval. If not, one can simply re–scale the equations so that the interval is of unit length. We have shown that the eigenvalues in one dimension are of the form

$$k_n^2 = n^2 \pi^2.$$

For diffusion–driven instability to occur we require that the Turing conditions (28)–(31) are satisfied and that

$$\gamma L = k_-^2 < k_n^2 < k_+^2 = \gamma R \tag{51}$$

where L and R are defined in (41) and (42). The inequality (51) is necessary but not sufficient for selection of say, a particular excitable wavenumber.

Selection of parameter values in one dimension

If we wish to isolate this mode, an additional condition is that

$$k_{n-1}^2 < k_-^2 < k_n^2 < k_+^2 < k_{n+1}^2. \tag{52}$$

Recall that when we calculated the homogeneous steady state for each model, we fixed all other parameters except for γ and d. We chose d as bifurcation parameter. Therefore, if we fix $d\,(> d_c)$ and vary γ, then (51) allows us to calculate which modes will have positive growth rate, while (52) can be used to help us to isolate modes for given parameter values satisfying inequalities (28)–(31).

Selection of parameter values in one dimension

The first derivatives of f and g evaluated at $(1.0, 0.9)$ are given by

$$f_u = \frac{b-a}{a+b} = 0.8, \qquad f_v = (a+b)^2 = 1.0, \tag{53}$$

$$g_u = \frac{-2\,b}{a+b} = -1.8, \qquad g_v = -(a+b)^2 = -1.0. \tag{54}$$

The critical diffusion coefficient ratio satisfies the quadratic equation

$$(d_c f_u + g_v)^2 = 4\,d_c\,(f_u\,g_v - f_v\,g_u). \tag{55}$$

Substituting leads to

$$0.64\,d_c^2 - 5.6\,d_c + 1 = 0 \tag{56}$$

from which we obtain the roots $d_c = 0.1824$ and 8.5676. But from linear stability analysis $d > 1$. Therefore we take the critical diffusion coefficient ratio as $d_c = 8.5676$. For illustrative purposes we take $d = 10$.

Isolation of excitable wave numbers

Gierer–Meinhardt γ	Thomas γ	Schnakenberg γ	Wavenumbers excited
0 – 58	0 – 20	0 – 19	–
59 – 82	21 – 46	20 – 49	$k_1 = \pi$
83 – 234	47 – 80	50 – 78	–
235 – 328	81 – 181	79 – 177	$k_2 = 2\pi$
329 – 526	182 – 185	178 – 197	$k_2 = 2\pi, k_3 = 3\pi$
527 – 739	186 – 323	198 – 315	$k_3 = 3\pi$
740 – 936	324 – 418	316 – 444	$k_3 = 3\pi, k_4 = 4\pi$
937 – 1314	419 – 505	445 – 493	$k_4 = 4\pi$
1315 – 1462	506 – 727	494 – 710	$k_4 = 4\pi, k_5 = 5\pi$
1463 – 2053	728 – 990	711 – 789	$k_4 = 4\pi, k_5 = 5\pi, k_6 = 6\pi$

Selection of parameter values in two dimensions

We are interested in determining both γ and d in isolating particular wavenumbers. We consider a unit square. The eigenvalues of the Laplacian take the form

$$k_{m,n}^2 = \pi^2\left(m^2 + n^2\right). \tag{57}$$

The parameter values must satisfy conditions (28)–(31) and also the conditions that

$$k_{max}^2 < \gamma L = k_-^2 < k_{m,n}^2 = \pi^2(m^2 + n^2) < k_+^2 = \gamma R < k_{min}^2 \tag{58}$$

where

$$k_{max}^2 = \max\{\forall k_{p,q}^2 : k_{p,q}^2 < k_{m,n}^2\}, \tag{59}$$

$$k_{min}^2 = \min\{\forall k_{p,q}^2 : k_{p,q}^2 > k_{m,n}^2\}. \tag{60}$$

Selection of parameter values in two dimensions

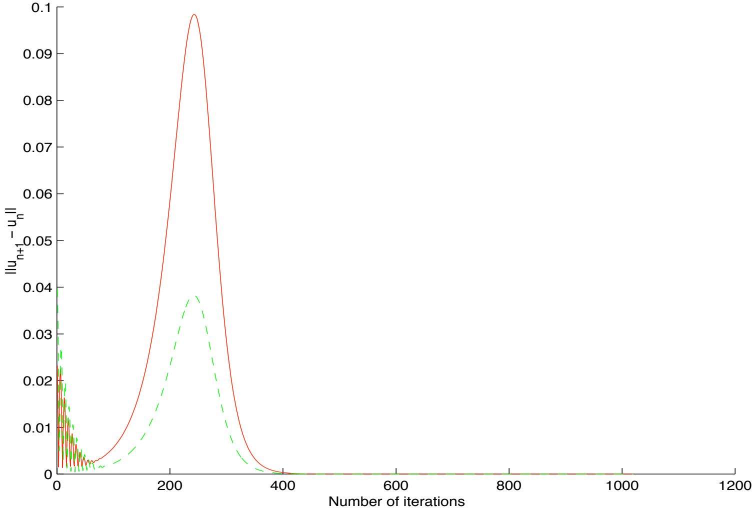
We impose the lower (k^2_{max}) and upper (k^2_{min}) bounds on k^2_- and k^2_+ respectively so that $k^2_{m,n}$ will be the only eigenvalue for which $\mathrm{Re}\lambda(k^2) > 0$ (see Figure for illustration). L and R are defined as in the one–dimensional case and are in fact independent of the dimension of the system. There are two roots to relation (23), hence we plot the real part of the larger root. The implementation of these conditions is based on the following algorithm:

1. If $k^2_- > k^2_{m,n}$ or $k^2_+ > k^2_{min}$ then decrease the value of γ by 0.01 and define $d = d_c + \epsilon$ where ϵ is a positive small parameter, thereby shifting the dispersion curve to the left.
2. Else if $k^2_+ < k^2_{m,n}$ or $k^2_- < k^2_{max}$ then increase the value of γ by 0.01 and $d = d_c + \epsilon$ is defined as above, shifting the curve to the right.

Selection of parameter values in two dimensions

Mode	Gierer–Meinhardt		Thomas		Schnakenberg	
(m,n)	d	γ	d	γ	d	γ
(1,0)	520.1573	67	427.0152	44	10	29
(1,1)	105.1573	168.8	39.0152	79	11.5776	70.6
(2,0)	84.1573	238.26	54.0152	122	10	114
(2,1)	77.6473	411.42	29.0152	170	9.1676	176.72
(2,2)	75.1573	483.43	30.9152	252	8.6676	230.82
(3,0)	70.8473	619.45	36.0152	269	8.6176	265.22
(3,1)	72.1573	756.23	27.5152	320	8.6676	329.20
(3,2)	73.1573	901.38	28.4152	402	8.8676	379.21
(3,3)	70.5573	1266.99	28.5152	553	8.6076	535.09

Linear predictions vs Numerical Solutions



Linear predictions vs Numerical Solutions