

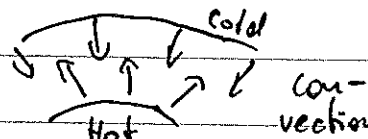
Pattern Formation

PREPARED BY

DATE

Pattern in nature form at all levels of organization:

- spirals of stars in galaxies
- weather patterns on earth (hurricanes)
- sand ripples and sand dunes \rightarrow flow + friction; but granular dynamics
- icicles, snowflakes \rightarrow gravity, water/heat diffusion
- stone models
- animal coat patterns



\Rightarrow all systems that are driven out of equilibrium
(flux of heat, mass, momentum, energy)

\rightarrow cells exchange ions/molecules

in contrast: equilibrated systems correspond to vanishing fluxes
hence system must be spatially uniform (featureless)

2nd law of thermodynamics implies that an isolated system always evolves towards a state of largest entropy

That state is the equilibrium (uniform) state. $\frac{dS}{dt} \geq 0$

In order for patterns to form (i.e. entropy falls) the system needs an external sink of entropy (environment generating ext. fluxes).

Therefore, the process of pattern formation can be generally understood as the result of competition between the external driving fluxes lowering the entropy and the internal dissipating fluxes raising the entropy.

Most natural systems are difficult to study and understand.

\Rightarrow use highly simplified laboratory experiments that can be carefully controlled and have lots of resemblance with natural phenomena to make quantitative/mathematical progress.

Most prominent examples are Rayleigh-Bénard Convection (rice cooker) and Belousov-Zhabotinsky reaction (spirals).

Perhaps the most magical moment is when pattern first appears "out of nothing", i.e. uniform state, no structure. As system is driven further and further out of equilibrium (by some experimental "kicks"), a point is eventually reached where small perturbations grow (instead of decay as they would if dissipation was stronger) and a non-uniform spatial structure appears.

Both uniform featureless state and pattern are stable states (steady state) solutions.

⇒ use linear stability analysis to understand pattern forming process.

One of the most interesting biologically relevant applications are reaction-diffusion systems. Historically, Alan Turing first carried out such a linear stability analysis in the context of reacting and diffusing chemicals to explain morphogenesis. (emergence of biological patterns in developing organism).

A chemical Turing system does not represent any real chemical system, it only describes the mechanism of the instability that leads to pattern formation. The phenomena discovered by Turing termed "diffusion-driven instability" is very general and found across many disciplines.

Recap: Stability of ODE's stationary state in 2D

$$\begin{cases} \partial_t u = f(u, v) \\ \partial_t v = g(u, v) \end{cases} \quad \text{with stationary state } (u_0, v_0) \quad \begin{cases} f(u_0, v_0) = 0 \\ g(u_0, v_0) = 0 \end{cases}$$

→ linear stability analysis: $u = u_0 + \delta u$
 $v = v_0 + \delta v$

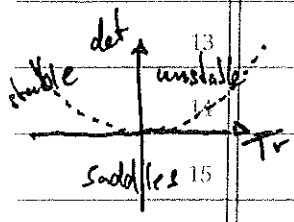
using $f(u, v) = f(u_0, v_0) + \delta u \frac{\partial f}{\partial u}(u_0, v_0) + \delta v \frac{\partial f}{\partial v}(u_0, v_0) + \dots$ (higher order)

$$\Rightarrow \begin{cases} \partial_t \delta u = \partial_u f \delta u + \partial_v f \delta v \\ \partial_t \delta v = \partial_u g \delta u + \partial_v g \delta v \end{cases}$$

→ look for solutions of the linearised system in form of simple exp

$$\delta u = \delta \bar{u} e^{w t} \quad \text{and} \quad \delta v = \delta \bar{v} e^{w t}$$

$$\Rightarrow \begin{cases} w \begin{pmatrix} \delta \bar{u} \\ \delta \bar{v} \end{pmatrix} = \begin{pmatrix} \partial_u f & \partial_v f \\ \partial_u g & \partial_v g \end{pmatrix} \begin{pmatrix} \delta \bar{u} \\ \delta \bar{v} \end{pmatrix} \end{cases} \quad \begin{array}{l} \text{character.} \\ \text{eg. } \rightarrow w^2 - w \text{Tr} + \text{det} = 0 \end{array}$$



obtain stability of stationary state if $\text{Re}(w) < 0$

$$\Rightarrow \text{Tr} = \partial_u f + \partial_v g < 0 \quad \text{and} \quad \text{det} = \partial_u f \partial_v g - \partial_v f \partial_u g > 0$$

The Turing model for two reacting ($f(u, v)$ and $g(u, v)$) and diffusing (D_u and D_v) species of chemicals is given by:

$$\begin{cases} \partial_t u = f(u, v) + D_u \partial_x^2 u \\ \partial_t v = g(u, v) + D_v \partial_x^2 v \end{cases} \quad \text{or} \quad \partial_t \vec{u} = \vec{f}(\vec{u}) + D \partial_x^2 \vec{u}$$

Assume stationary uniform state (u_0, v_0) and linearize to obtain perturbation dynamics:

$$\begin{aligned} \partial_t \delta u &= \partial_u f \delta u + \partial_v f \delta v + D_u \partial_x^2 \delta u + \dots \quad (\text{h.o.}) \\ \partial_t \delta v &= \partial_u g \delta u + \partial_v g \delta v + D_v \partial_x^2 \delta v + \dots \quad (\text{h.o.}) \end{aligned}$$

$$\text{or } \partial_t \begin{pmatrix} \delta u \\ \delta v \end{pmatrix} = \underbrace{\left(A + D \partial_x^2 \right)}_{\text{Jacobian}} \begin{pmatrix} \delta u \\ \delta v \end{pmatrix} \quad \text{with } A = \begin{pmatrix} \partial_u f & \partial_v f \\ \partial_u g & \partial_v g \end{pmatrix}$$

Let's try the solution $\delta u_f = \delta \bar{u}_f e^{\omega_f t} e^{iqx}$
 $\delta v_f = \delta \bar{v}_f e^{\omega_f t} e^{iqx}$ } "noise" perturbations
 f -modes

to obtain the eigenvalue problem: $A_f \begin{pmatrix} \delta u_f \\ \delta v_f \end{pmatrix} = \omega_f \begin{pmatrix} \delta u_f \\ \delta v_f \end{pmatrix}$

with $A_f \equiv A - q^2 D = \begin{pmatrix} \partial_u f - q^2 D_u & \partial v f \\ \partial_u g & \partial v g - q^2 D_v \end{pmatrix}$

The solution to the linearized perturbation dynamics is then

$$\begin{pmatrix} \delta u \\ \delta v \end{pmatrix} = \begin{pmatrix} c_1 \begin{pmatrix} \delta u_f^{(1)} \\ \delta v_f^{(1)} \end{pmatrix} e^{\omega_f^{(1)} t} + c_2 \begin{pmatrix} \delta u_f^{(2)} \\ \delta v_f^{(2)} \end{pmatrix} e^{\omega_f^{(2)} t} \end{pmatrix} e^{iqx}$$

Notes: in ω, ω^2
 and $\omega^{(i)}$ the
 exponents are
 indices, not
 potentialities

with $\begin{pmatrix} \delta u_f^{(i)} \\ \delta v_f^{(i)} \end{pmatrix}$ and $\omega_f^{(i)}$ eigen vectors and ω -values of A . Instability of the uniform state implies $\max_{i,q} \text{Re}(\omega_f^{(i)}) > 0$.

To analyze stability let's determine when the real parts of both eigenvalues are negative:

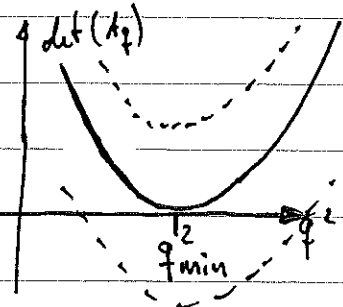
- ① $\omega_f^1 + \omega_f^2 = \text{Tr}(A_f) = \partial_u f + \partial_v g - q^2(\partial_u + \partial_v) < 0$
- ② $\omega_f^1 \cdot \omega_f^2 = \det(A_f) = (\partial_u f - q^2 \partial_u)(\partial_v g - q^2 \partial_v) - \partial v f \partial_u g > 0$

If the diffusion of chemicals is to cause an instability, then the reacting chemicals form a stable uniform state when no diffusion is present. Hence for $D_u = D_v = 0$, stability requires (from ① and ②):

$$\partial_u f + \partial_v g < 0 \quad \text{and} \quad \partial v f \partial_u g - \partial_u f \partial_v g > 0$$

Therefore ① is automatically satisfied ($D_u > 0$ and $D_v > 0$) and so the modes $\delta u_f^{(i)} e^{iqx}$ become marginally stable (i.e. $\text{Re}(\omega_f^{(i)}) = 0$) when

② $\det A_f = 0$



At q_{\min} is the first mode that can cause instability.

$$q_{\min}^2 = \frac{D_u \partial_v g + D_v \partial_u f}{2 D_u D_v}$$

$$\det A_f|_{q_{\min}} = \partial_u \partial_v g - \partial_u f \partial_v g - \frac{(D_u \partial_v g - D_v \partial_u f)^2}{4 D_u D_v} > 0$$

Stability requires $\det A_q > 0 \quad \forall q$, hence the onset of instability corresponds to $\det A_q|_{q_{min}}$ becoming negative.

$$\Rightarrow \boxed{D_u \partial_{xx}^2 + D_v \partial_{xx}^2 > 2 \sqrt{D_u D_v} (\partial_{uf} \partial_{vg} - \partial_{uf} \partial_{vf})} \Leftrightarrow \boxed{\text{Turing instability}} \quad (3)$$

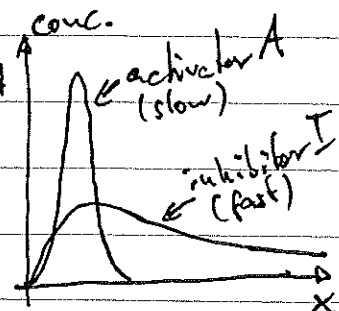
$$(3) \Rightarrow \left. \begin{array}{l} D_u \partial_{xx}^2 + D_v \partial_{xx}^2 > 0 \\ \text{together with } D_u > 0, D_v > 0, \text{ and } (1) \end{array} \right\} \begin{array}{l} \partial_{uf} \text{ and } \partial_{vg} \text{ have opposite} \\ \text{signs} \end{array}$$

Hence one of the chemicals (say u) should act as its own catalyst (enhance its own rate of production, $\partial_{uf} > 0$), while the other should act as its own inhibitor. This is called an activator-inhibitor system.

The necessary instability condition $\frac{D_v}{D_u} > -\frac{\partial_{vg}}{\partial_{uf}} > 0$ implies that the ratio of Diffusion constants has to exceed $\frac{\partial_{vg}}{\partial_{uf}}$ the ratio of reaction rates, often referred to as "local activation with long-range inhibition". Since diffusion constants for simple chemicals in solution are similar, this condition is hard to satisfy \Rightarrow Turing instabilities are rare...
reaction rates or lifetimes

The wavelength of the establishing pattern after instability is given by $\frac{1}{q_{min}}$. At the instability, microscopic noise with the right q will be amplified by the system and spontaneously emerges a spatial pattern with the matching wavelength $\lambda = \frac{1}{q}$.

Intuitively, noise fluctuation of slowly diffusing activator A grows into a peak, activating inhibitor I that diffuses away rapidly, inhibition further activator fluctuations to grow nearby, generating a "ring" of no pattern. If I doesn't diffuse away, peak A cannot grow...



Generally linear stability analysis will reveal a most unstable wavelength (perturbations ("noise") with this wavelength grow fastest), and this is generally a good guide for the final pattern. Note that details of final pattern depend on boundary conditions (more than on actual forms of $f(u,v)$ and $g(u,v)$) and on initial conditions. The latter can be problematic if consistent and reproducible pattern is desired, such as for morphogenesis \Rightarrow Turing mechanism rarely employed for embryonic development...

Example: Chemical reaction-diffusion model (Brusselator)

$$f(u,v) = a - (b+1)u + u^2v$$

$$g(u,v) = bu - u^2v$$

with bifurcation parameter $b > 0$ and $a = 1.5$, $D_u = 2.8$, $D_v = 22.4$

Steady state $(u_0, v_0) = (a, \frac{b}{a})$

Jacobian $A = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix}$

Stability in the absence of Diffusion:

$$\det A = -a(b^2 + a^2) + a^2b = a^2 > 0$$

$$\text{Tr } A = b - 1 - a^2 < 0 \quad \Rightarrow \quad b < b_0 = 1 + a^2 = 3.25$$

Instability in the presence of Diffusion:

$$D_u A_{22} + D_v A_{11} > 2 \sqrt{D_u D_v (A_{11} A_{22} - A_{12} A_{21})}$$

$$\Rightarrow D_u(-a^2) + D_v(b-1) > 2 \sqrt{D_u D_v a^2}$$

$$\Rightarrow b > 1 + \frac{1}{D_v} (2a \sqrt{D_u D_v} + a^2 D_u) = \left(1 + \sqrt{\frac{D_u}{D_v}} a\right)^2 = b_c = 2.34$$

\Rightarrow Turing instability only arises for $b_c < b < b_0$

At onset, $b = b_c$, the critical wavenumber is given by $q_c = q_{\min} = \frac{\sqrt{D_v(b-1) - D_u a^2}}{2 \sqrt{D_u D_v}}$

which corresponds to a spatially periodic pattern with

period $\lambda = \frac{2\pi}{q_c} \approx 14.5$