Tutorial on Turing instability and pattern formation

Duccio Fanelli

Dipartimento di Fisica e Astronomia, Università degli Studi di Firenze
CSDC – Centro Interdipartimentale per lo Studio delle Dinamiche Complesse
INFN – Istituto Nazionale di Fisica Nucleare, Sezione di Firenze

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Patterns formation in nature

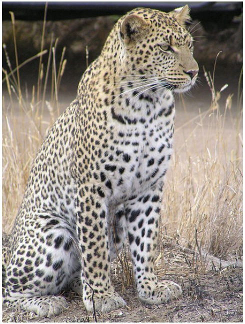
Investigating the dynamical evolution of an ensemble made of microscopic entities in mutual interaction constitutes a rich and fascinating problem, of paramount importance and cross-disciplinary interest (biology, ecology, physics, chemistry).

- Complex microscopic interactions can eventually yield to macroscopically organized patterns.
- Temporal and spatial order manifests as an emerging property of the system dynamics

Self-organized phenomena are ubiquitous in nature

A system is said to self-organized when...

- ..it is composed by a large set of homologous constituents
- ..regular, collective feautures emerge spontaneously.



The Belousov-Zhabotinsky reaction.

Highlighting the peculiarities:

- First system to display self-organization
- Regular oscillations between homogeneous states.

Experimental evidence

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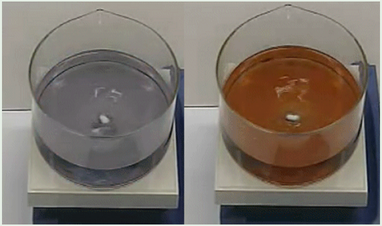

Belousov e Zhabotinsky
Med. Publ. Moscow (1959) - *Biofizika* (1964)

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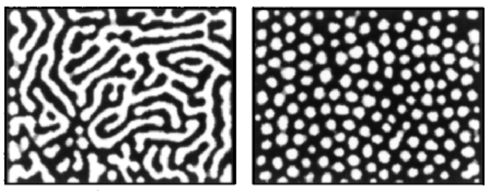

Spatially organized patterns develop (Turing instability) - Vanag e Epstein *Phys. Rev. Lett.* (2001)

Alan Turing (1912-1954)

1. Turing machine, a general purpose computer: concepts of algorithm and computation with the Turing machine.
2. Pivotal role in cracking intercepted coded messages during II world war.
3. Mathematical biology: chemical basis of morphogenesis.

Morphogenesis

Morphogenesis is the biological process that causes an organism to develop its shape.

Morphogenesis addresses the problem of biological form at many levels, from the structure of individual cells, through the formation of multicellular arrays and tissues, to the higher order assembly of tissues into organs and whole organisms.

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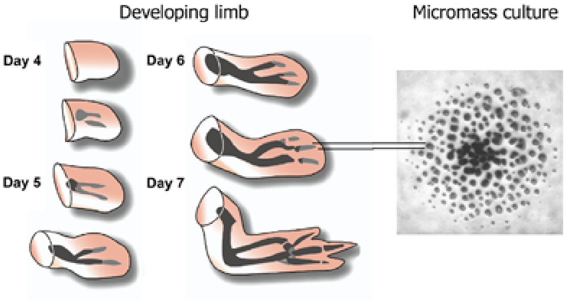
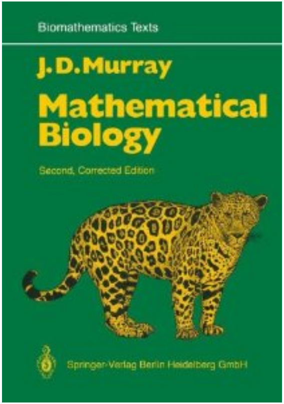


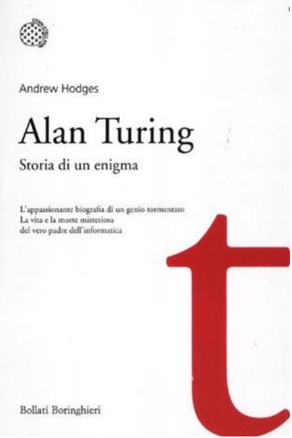
The complete and fine detailed understanding of the mechanisms involved in actual organisms required the discovery of DNA and the development of molecular biology and biochemistry.

Although the mechanism must be genetically controlled , the genes themself cannot create the patterns. They only provide a blue print or recipe, for the pattern generation.

Turing suggested that under certain conditions, chemicals can react and diffuse in such a way as to produce steady state heterogeneous spatial patterns of chemical or morphogen concentration.

Two books


Biomathematics Texts
J. D. Murray
Mathematical Biology
Second, Corrected Edition
Springer-Verlag Berlin Heidelberg GmbH


Andrew Hodges
Alan Turing
Storia di un enigma
L'appassionante biografia di un genio tormentato
La vita e la morte misteriosa
del vero padre dell'informatica
Bollati Boringhieri

Model the dynamics of the population involved (family of homologous chemicals)

From the microscopic picture ...

- Assign the microscopic rules of interactions
- Discrete, many particles model

Deterministic formulation (continuum limit hypothesis)

- Differential equations
- No fluctuations allowed

Stochastic model (respecting the intimate discreteness)

- Stochastic processes
- Statistical, finite sizes fluctuations

The deterministic (continuum) picture

The law of mass action

From chemical equations to ordinary differential equations:

$$X \xrightarrow{\lambda} \emptyset \qquad \Longrightarrow \qquad \dot{\phi} = -\lambda\phi$$

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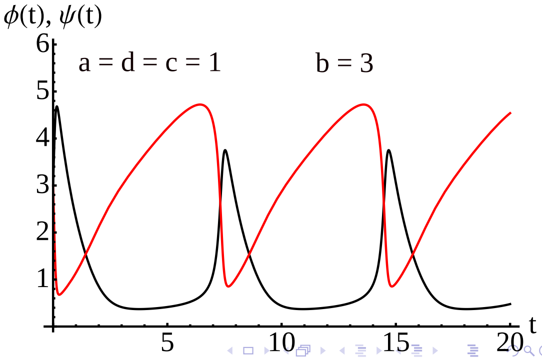
The a-spatial Brusselator

Continuum concentration

$$\begin{cases} \phi = \phi(t) & \text{species } X \\ \psi = \psi(t) & \text{species } Y \end{cases}$$

Equations

$$\begin{cases} \dot{\phi} = a - (b+d)\phi + c\phi^2\psi \\ \dot{\psi} = b\phi - c\phi^2\psi \end{cases}$$



Deterministic reaction-diffusion systems

Alan Turing

The Turing instability (1952)

$$
\begin{aligned}
\partial_t \phi &= f(\phi, \psi) + D_\phi \, \nabla^2 \phi \\
\partial_t \psi &= g(\phi, \psi) + D_\psi \, \nabla^2 \psi
\end{aligned}
$$

where:

1. $\phi(\mathbf{r}, t)$ and $\psi(\mathbf{r}, t)$ are the species concentrations.
2. D_ϕ and D_ψ denote the diffusion coefficients

An informative albeit unrealistic image (Murray) (1)

1. Consider a field of dry grass with a large number of grasshoppers which can generate moisture by sweating if they get warm.
2. Suppose the grass is set alight at some point and the front starts to propagate.
3. When the grasshoppers get warm enough they can generate enough moisture to dampen the fire: when the flames will reach the pre-moistened area the grass will not burn.

An informative albeit unrealistic image (Murray) (2)

1. The fire starts to spread. When the grasshoppers ahead of the flame front feel it coming they move well ahead of it ($D_G > D_F$).
2. The grasshoppers sweat profusely, generate moisture and prevent the fire to spread into the moistened area.
3. The burned area is hence restricted to a given domain which depends on the parameters of the game.
4. If instead of a initial single fire there was a random scattering of them, the process would result in a final spatially inhomogeneous distribution of burnt and preserved patches.
5. Notice that the inhibitors (grasshopers) diffuse faster the the activator (fire).

I. Stable fixed point of the aspatial model

Assume a stable homogeneous fixed point of the dynamics to exist and label it (ϕ^*, ψ^*):

$$
\begin{aligned}
f(\phi^*, \psi^*) &= 0 \\
g(\phi^*, \psi^*) &= 0
\end{aligned}
$$

The Jacobian matrix

$$
\mathcal{J} = \begin{pmatrix} f_\phi & f_\psi \\ g_\phi & g_\psi \end{pmatrix}
$$

The stability of the fixed point implies $\mathrm{Tr}\,\mathcal{J} < 0$ and $\det \mathcal{J} > 0$.

II. The perturbation.

Introduce a small non homogeneous perturbation of the fixed point:

$$\mathbf{w} = \begin{pmatrix} \phi - \phi^* \\ \psi - \psi^* \end{pmatrix}.$$

and linearize the reaction-diffusion equations to get:

$$\dot{\mathbf{w}} = \mathcal{J}\mathbf{w} + \mathbf{D}\nabla^2\mathbf{w},$$

where

$$\mathbf{D} = \begin{pmatrix} D_\phi & 0 \\ 0 & D_\psi \end{pmatrix}.$$

III. Laplacian's eigenfunctions

To solve the linearized system one introduces $\mathbf{W}_k(\mathbf{x})$ such that:

$$\nabla^2 \mathbf{W}_k(\mathbf{x}) = -k^2 \mathbf{W}_k(\mathbf{x}),$$

Expand the perturbation **w** as

$$\mathbf{w}(\mathbf{x}, t) = \sum_{k \in \sigma} c_k e^{\lambda(k) t} \mathbf{W}_k(\mathbf{x}),$$

1. c_k refer to the initial condition.
2. Equivalent to Fourier transforming the original equation.
3. $\lambda(k)$ defines the dispersion relation

Substituting the ansatz in the linear system yields:

$$\lambda \mathbf{W}_k = \mathcal{J}\mathbf{W}_k - k^2 \mathbf{D}\mathbf{W}_k$$

or equivalently:

$$\begin{pmatrix} f_\phi - D_\phi k^2 - \lambda & f_\psi \\ g_\phi & g_\psi - D_\psi k^2 - \lambda \end{pmatrix} \mathbf{W}_k = 0$$

We require non trivial solutions for $\mathbf{W}_k$ which implies that λ is determined by the roots of the characteristic polynomial:

$$det(\lambda(k)\mathbf{I} - \mathcal{J} - \mathbf{D}k^2) = 0$$

The Turing instability occurs if one can isolate a finite domain in k for which $\mathrm{Re}(\lambda(k)) > 0$.

A simple calculation (done on the blackboard) yields the following general condition for the Turing instability to sets in:

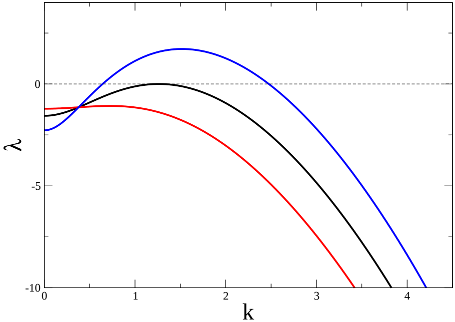
$$\begin{aligned}(D_\phi g_\psi + D_\psi f_\phi)^2 &> 4 D_\phi D_\psi (f_\phi g_\psi - f_\psi g_\phi) \\ (D_\phi g_\psi + D_\psi f_\phi) &> 0\end{aligned}$$

which sum up to the aforementioned conditions:

$$f_\phi + g_\psi < 0 \qquad\qquad f_\phi g_\psi - f_\psi g_\phi > 0$$

Important remarks

1. f_ϕ and g_ψ must be of opposite sign.
2. Assume $f_\phi > 0$ (activator) and $g_\psi < 0$ (inhibitor). Then, $f_\phi + g_\psi < 0$ implies:
$$f_\phi < |g_\psi|$$
and thus:
$$\frac{D_\psi}{D_\phi} > \frac{|g_\psi|}{f_\phi} > 1$$
the inhibitor must diffuse faster than the activator.
3. Boundary conditions do matter.

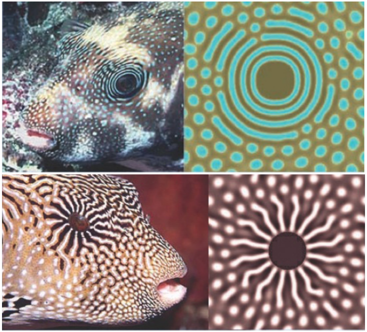


1. Species ϕ is the activator,
2. ψ play the role of the inhibitor.

$$
\begin{aligned}
f(\phi,\psi) &= a-(b+d)\phi+c\phi^2\psi \\
g(\phi,\psi) &= b\phi-c\phi^2\psi
\end{aligned}
$$

From a random perturbation of the homogeneous fixed point to a stationary pattern.

Turing patterns are widespread



I. Patterns on a (symmetric) network.

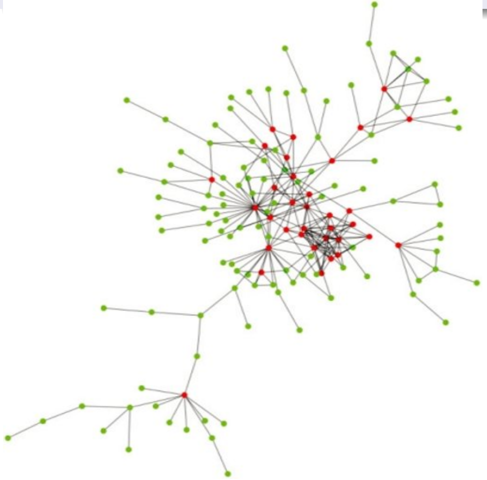
Adjacency matrix

$$\mathbf{W} = \begin{bmatrix} 1 & 0 & 0 & \cdots & \\ \cdots & & 0 & 1 & \cdots \\ \vdots & \vdots & \cdots & \vdots & \\ \cdots & 1 & 0 & 1 & \cdots \end{bmatrix}$$

$W_{ij} = 1$, if nodes i and j are connected ($i \neq j$), and $W_{ij} = 0$ otherwise

$$k_i = \sum_{j=1}^{\Omega} W_{ij} \quad \text{(node degree)}$$

Scale-free network



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Reaction-diffusion equations

$$\begin{aligned} \partial_t \phi_i &= f(\phi_i, \psi_i) + D_\phi \sum_{j=1}^{\Omega} L_{ij} \phi_i \\ \partial_t \psi_i &= g(\phi_i, \psi_i) + D_\psi \sum_{j=1}^{\Omega} L_{ij} \psi_i \end{aligned}$$

where $i = 1, .., \Omega$ and $L_{ij} = W_{ij} - k_i \delta_{ij}$ is the discrete Laplacian operator.

Linear stability analysis on networks

Perturbation near the homogeneous fixed point

$$\phi_i = \phi^* + \delta\phi_i \quad \psi_i = \psi^* + \delta\psi_i$$

- Linearize the equations for ϕ_i and ψ_i
- Introduce the eigenvectors of the Laplacian

$$\sum_j L_{ij}\Phi_j^{(\alpha)} = \Lambda^{(\alpha)}\Phi_i^{(\alpha)}$$

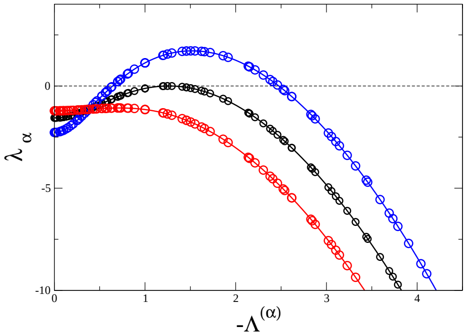
The eigenvalues $\Lambda^{(\alpha)}$ are real and negative.

The set of eigenvectors define a basis on which we can expand the perturbation.

$$\delta\phi_i = \sum_{\alpha=1}^{\Omega} c_\alpha e^{\lambda_\alpha \tau}\Phi_i^{(\alpha)}$$
$$\delta\psi_i = \sum_{\alpha=1}^{\Omega} c_\alpha \beta_\alpha e^{\lambda_\alpha \tau}\Phi_i^{(\alpha)}$$

Inserting in the linearized equation one gets a dispersion relation for λ_α versus $\Lambda^{(\alpha)}$, which controls the instability.

Dispersion relation for the Brusselator model



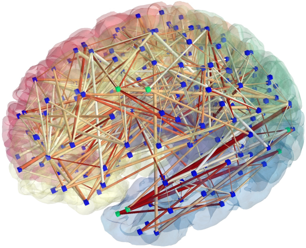
The dispersion relation is defined on the discrete support of Ω eigenvalues $\Lambda^{(\alpha)}$.

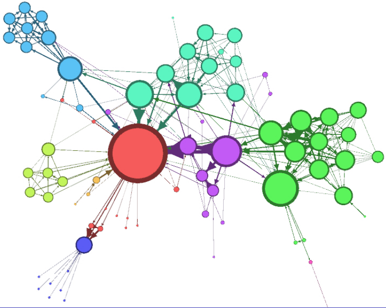
The curve relative to the continuum case is recovered by replacing $\Lambda^{(\alpha)}$ with $-k^2$.

A segregation in activator/inhibitors rich/poor nodes is found as follows the linear instability.

Adjacency matrix

- In this case the adjacency matrix is asymmetric, hence $W_{ij} \neq W_{ji}$
- Due to the asymmetry the spectra of the Laplacian $\Lambda^{(\alpha)}$ are complex.
- The dispersion relation can turn unstable also when it is stable on a symmetric support.





From the linear stability analysis...

In analogy with the above:

$$\mathcal{J}_\alpha = \mathcal{J} + \mathbf{D}\Lambda^{(\alpha)}$$

whose eigenvalues are such that:

$$(\lambda_\alpha)_{Re} = \frac{1}{2}\left[(\mathrm{tr}\mathcal{J}_\alpha)_{\mathrm{Re}} + \gamma\right]$$

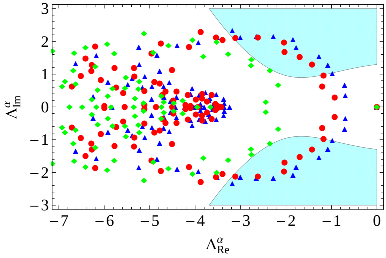
where γ is a functions of $\mathcal{J}_\alpha$

Region of instability

The instability develops when $(\lambda_\alpha)_{Re}$ is positive, namely when:

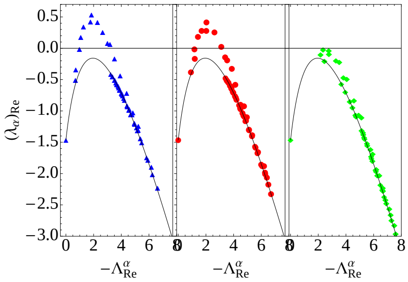
$$S_2(\Lambda^{(\alpha)}_{\mathrm{Re}})\left[\Lambda^{(\alpha)}_{\mathrm{Im}}\right]^2 \le -S_1(\Lambda^{(\alpha)}_{\mathrm{Re}}),$$

where S_1 and S_2 are polynomials of fourth and second degree in $\Lambda^{(\alpha)}_{\mathrm{Re}}$

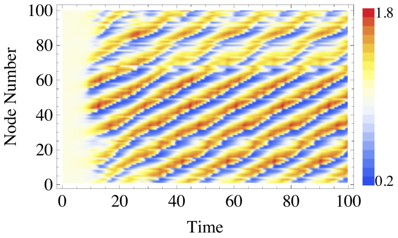


The instability region (shaded) in the $(\Lambda^{(\alpha)}_{\mathrm{Re}}, \Lambda^{(\alpha)}_{\mathrm{Im}})$ plane.

Dispersion relations for Newman-Watts networks with different p, the probability of long-range links



Self-organized waves can develop instigated by the network topology.



M. Asllani et al, Nature Communications (2014)

Stationary (Turing) patterns are also obtained when changing p.