Phenomenology of Reaction-Diffusion Systems

Since $\sigma = \sigma(k^2)$ (by left-right symmetry), we would require

$$\sigma(k) \sim \alpha + \beta k^2 - \gamma k^4 + \ldots$$
$$u_t = \alpha u - \beta u_{xx} - \gamma u_{4x} + \ldots$$

but such higher-order derivative theories for a single degree of freedom are rare. Instead, two *coupled* reaction-diffusion equations can produce this behavior.

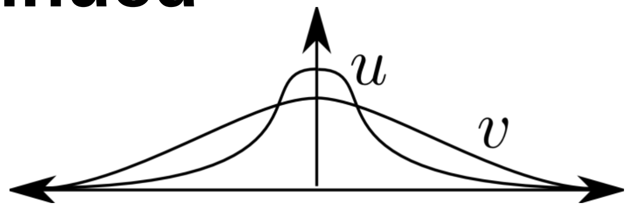
The FitzHugh-Nagumo model. The FHN model was first developed as a simplification neuronal dynamics. Two chemical species are involved: u, the *activator*, and v, the inhibitor. Under suitable rescalings it typically takes the form

$$u_t = D\nabla^2 u + f(u) - \rho v$$
$$\epsilon v_t = \nabla^2 v + \alpha u - \beta v \ .$$

Notice that the inhibitor diffusion constant has been rescaled to unity. We may be interested in a whole range of values for ϵ, not necessarily small. The various terms on the RHS of the equations are:

$f(u)$	Autocatalysis & bistability
ρv	Inhibition
αu	Stimulation
βv	Self-limitation

FHN Model - continued



The presence of the relative diffusion constant D can produce *lateral inhibition* for $D \ll 1$ (different length scales).

Depending on the terms f, D, ϵ, the FHN model can produce homogeneous states, strips, or other periodic patterns, spiral waves, etc.

It is sometimes useful to write the FHN model in a more symmetric form

$$
\begin{aligned}
u_t &= D\nabla^2 u + f(u) - \rho(v-u) \\
\epsilon v_t &= \nabla^2 v + u - v
\end{aligned}
$$

Does this model have any definite variational structure? Many of the terms conform to a gradient flow:

$$
\begin{aligned}
u_t &= -\frac{\delta E_u}{\delta u} - \rho v \\
\epsilon v_t &= -\frac{\delta E_v}{\delta v} + u
\end{aligned}
$$

The remaining terms are actually Hamiltonian!

$$
u_t = -\rho v \qquad \epsilon v_t = u
$$

The Fast-Inhibitor Limit

Consider the simplest regime (like in Michaelis-Mentin kinetics), the *fast inhibitor limit*. Here we set $\epsilon = 0$ and obtain a local in time but nonlocal in space relationship between v and u:

$$(\nabla^2 - 1)v = -u$$

Given a Green's function for the operator $(\nabla^2 - 1)$, we can solve this:

$$v(\mathbf{x}) = \int d\mathbf{x}' G(\mathbf{x} - \mathbf{x}') u(\mathbf{x}')$$

For example, in one dimension,

$$G(x - x') = \frac{1}{2} \mathrm{e}^{-|x - x'|}$$

and in two dimensions,

$$G(\mathbf{x} - \mathbf{x}') = \frac{1}{2\pi} K_0(|\mathbf{x} - \mathbf{x}')$$

So, in the fast inhibitor limit we have

$$u_t = D\nabla^2 + f(u) + \rho u - \rho \int d\mathbf{x}' G(\mathbf{x} - \mathbf{x}') u(\mathbf{x}')$$

which is a closed, nonlocal equation of motion. In fact, u is variational,

$$u_t = -\frac{\delta E}{\delta u}, \quad E = \int d\mathbf{x} \left\{ \frac{1}{2} D |\boldsymbol{\nabla} u|^2 + F(u) - \frac{1}{2}\rho u^2 \right\} + \frac{1}{2}\rho \int d\mathbf{x} \int d\mathbf{x}' u(\mathbf{x}) G(\mathbf{x} - \mathbf{x}') u(\mathbf{x}')$$

The nonlocal term reminds us of electrostatics.

The Turing Instability - I

Consider a 2-species model, with concentrations $u(\mathbf{x},t)$ and $v(\mathbf{x},t)$ in a bounded domain $\mathcal{D}$. We assume Neumann boundary conditions of no flux in or out, so $\hat{\mathbf{n}} \cdot \boldsymbol{\nabla} u\Big|_{\partial\mathcal{D}} = \hat{\mathbf{n}} \cdot \boldsymbol{\nabla} v\Big|_{\partial\mathcal{D}} = 0$

The pair of reaction-diffusion equations is

$$\begin{aligned} u_t &= D_u \nabla^2 u + f(u,v) \\ v_t &= D_v \nabla^2 v + g(u,v) \ , \end{aligned}$$

where f and g are some smooth functions of their arguments, representing, for example, autocatalysis, feedback inhibition, etc.

We suppose that f and g are such that there exists a *stable*, uniform steady state (so $f(u_0,v_0) = g(u_0,v_0) = 0$), i.e. the Jacobian

$$J = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}$$

has

$$\mathrm{Tr} = f_u + g_v < 0 \quad \text{and} \quad \mathrm{Det} = f_u g_v - f_v g_u > 0$$

at (u_0, v_0).

The Turing Instability - II

These requirements arise from linearizing the equations of motion via $u = u_0 + \delta u$, $v = v_0 + \delta v$, to obtain the dynamics

$$\partial_t \begin{pmatrix} \delta_u \\ \delta_v \end{pmatrix} = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} \begin{pmatrix} \delta_u \\ \delta_v \end{pmatrix}$$

As this is a linear equation it has solutions of the form $\mathrm{e}^{\sigma t}$, and σ will be determined by the determinental condition

$$\begin{vmatrix} f_u - \sigma & f_v \\ g_u & g_v - \sigma \end{vmatrix}$$

This is just $\sigma^2 - \mathrm{Tr}\sigma + \mathrm{Det}$, with solutions $\sigma_\pm = (1/2)\left\{\mathrm{Tr} \pm \sqrt{\mathrm{Tr}^2 - 4\mathrm{Det}}\right\}$. For stability, we require the real part of both roots of σ to be negative. So, if $\mathrm{Tr} < 0$ the root in which we choose the negative sign in front of the square root is clearly negative. There are two cases that will allow the second root to be negative. If $0 < \mathrm{Det} < \mathrm{Tr}^2/4$ the square root is real but less then $|\mathrm{Tr}|$ and the root is negative, while for larger values of Det the square root yields an imaginary contribution, and still the real part of σ is negative.

The Turing Instability – III

Now we examine what happens when we perturb this *homogeneous* steady state with spatial-temporal variations, $u = u_0 + p(\mathbf{x}, t)$, $v = v_0 + q(\mathbf{x}, t)$, to obtain the dynamics

$$p_t = f_u p + f_v q + D_u \nabla^2 p$$
$$q_t = g_u p + g_v q + D_v \nabla^2 q \ ,$$

It is always possible to expand a function of $\mathbf{x}$ in the domain $\mathcal{D}$ as an infinite series of eigenfunctions of the (Helmholtz) equation

$$\nabla^2 w_k + \lambda_k^2 w_k = 0 \quad (\text{in } \mathcal{D})$$
$$\hat{\mathbf{n}} \cdot \boldsymbol{\nabla} w_k = 0 \quad (\text{on } \partial\mathcal{D})$$

For example, in $d = 1$ with $\mathcal{D} = [0, L]$, we have $w_k = \cos(k\pi x/L)$ and $\lambda_k = k\pi/L$. More generally, if we write

$$p = \sum_k \hat{p}_k e^{\sigma_k t} w_k(\mathbf{x})$$
$$q = \sum_k \hat{q}_k e^{\sigma_k t} w_k(\mathbf{x})$$

and substitute (and drop the suffix “k”) for convenience,

The Turing Instability - IV

Then the new equation governing the growth rate will be similar to the homogeneous case, but with the diffusive contributions on the diagonal.

$$\begin{vmatrix} (f_u - D_u\lambda^2 - \sigma) & f_v \\ g_u & (g_v - D_v\lambda^2 - \sigma) \end{vmatrix} .$$

This will have a nontrivial solution if and only if

$$\sigma^2 + \left[(D_u + D_v)\lambda^2 - f_u - g_v\right]\sigma + (D_u\lambda^2 - f_u)(D_v\lambda^2 - g_v) - f_v g_u = 0$$

Now we note that the sum of the roots satisfies

$$\sigma_1 + \sigma_2 = -(D_u + D_v)\lambda^2 + f_u + g_v < 0 \ ,$$

where this negativity arises from the fact that the assumption of a stable *homogeneous* state already required $f_u + g_v < 0$, and the new diffusive contributions are clearly negative. The product of the two roots satisfies

$$\sigma_1\sigma_2 = D_u D_v \lambda^4 - (D_v f_u + D_u g_v)\lambda^2 + \mathrm{Det} \ ,$$

where Det is that of the homogeneous system.

The Turing Instability - V

To repeat:

$$\sigma_1\sigma_2 = D_u D_v \lambda^4 - (D_v f_u + D_u g_v)\lambda^2 + \text{Det} \ ,$$

Now, since the sum is < 0, one root can have a positive real part only if the product is < 0 (actually, then both roots are real). Thus, a *necessary* condition for instability is the possibility of a negative product, and since the λ^4 term is clearly positive and Det is positive, we require the overall coefficient of λ^2 be negative, or

$$D_v f_u + D_u g_v > 0 \ .$$

Without loss of generality, we can take $D_v > D_u > 0$. But if $f_u + g_v < 0$, we need f_u and g_v to have opposite signs, with $f_u > 0$ and $g_v < 0$. The condition above is not a sufficient condition for instability, since it must be possible to find a permitted λ that makes $\sigma_1\sigma_2 < 0$. That is, the equation (with $x = \lambda^2$)

$$h(x) = D_u D_v x^2 - (D_v f_u + D_u g_v)x + \text{Det} = 0$$

must have positive roots. This requires

$$(D_v f_u + D_u g_v)^2 > 4\text{Det} \cdot D_u D_v \ .$$

The Turing Instability - VI

Our sufficient condition is so provided one of the permitted λs lies between λ_- and λ_+,

$$\lambda_\pm^2 = \frac{1}{2D_uD_v}\left\{Dvf_u + D_ug_v \pm \sqrt{(D_vf_u + D_ug_v)^2 - 4D_uD_v\mathrm{Det}}\right\}$$

So our sufficient condition is

$$D_vf_u + D_ug_v > 2\sqrt{\mathrm{Det}}\sqrt{D_uD_v}$$

Now define $d = D_v/D_u > 1$. Then

$$df_u - 2\sqrt{\mathrm{Det}}\sqrt{d} + g_v > 0 \ .$$

This will clearly be true if d is sufficiently large. Looking at the crossing point (LHS=0) we find

$$\sqrt{d} = \frac{\sqrt{\mathrm{Det}} + \sqrt{\mathrm{Det} - f_ug_v}}{f_u}$$

So finally we can write the inequality (recall $f_ug_v < 0$)

$$\boxed{\sqrt{d} \geq \frac{1}{f_u}\left(\sqrt{\mathrm{Det}} + \sqrt{\mathrm{Det} - f_ug_v}\right) > 0 \ .}$$

The Turing Instability - VII

Finally, we can examine the typical length scale of the instability. At onset, $\lambda = \lambda_c$, where $h(\lambda_c^2) = 0$ is a double root. Then

$$D_v f_u + D_u g_v = 2\sqrt{\text{Det}}\sqrt{D_u D_v} \quad \text{and} \quad \lambda_c^2 = \frac{\sqrt{\text{Det}}}{\sqrt{D_u D_v}}$$

And then the unstable wavelength is

$$\ell_c = \frac{2\pi}{\lambda_c}$$

Let's look at an example (Murray, 1st edition, §14.2). Autocatalytic chemical reactions

$$\begin{aligned} u_t &= D_u \nabla^2 u + k_1 - k_2 u + k_3 u^2 v \\ v_t &= D_v \nabla^2 v + k_4 - k_3 u^2 v \ . \end{aligned}$$

This can be simplified by suitable rescalings. We can always find P, Q, R, S such that

$$\frac{\partial}{\partial t} \to P \frac{\partial}{\partial t} \ , \qquad u \to Qu \ , \qquad v \to Rv \ , \qquad \boldsymbol{\nabla} \to S\boldsymbol{\nabla} \ .$$

The Turing Instability - VIII

The result is the system

$$u_t = \nabla^2 u + a - u + u^2 v$$
$$v_t = d\nabla^2 v + b - u^2 v \ .$$

where as usual $d = D_v/D_u > 1$. With $f(u,v) = a - u + u^2 v$ and $g(u,v) = b - u^2 v$ the homogeneous fixed point is

$$u_0 = a + b \ , \qquad v_0 = \frac{b}{(a+b)^2} \ .$$

The Jacobian of the linear stability problem is then

$$\begin{pmatrix} (-1 + 2u_0 v_0) & u_0^2 \\ -2u_0 v_0 & -u_0^2 \end{pmatrix} .$$

Thus, $\mathrm{Tr} = -1 - u_0^2 + 2u_0 v_0$ and $\mathrm{Det} = u_0^2 > 0$. Substituting, we find

$$\mathrm{Tr} = \frac{b - a - (a+b)^3}{a+b} \ .$$

The Turing Instability - IX

Thus, the spatially uniform system is linearly stable is $b - a < (a+b)^3$. The *necessary* conditions are

$$f_u > 0 \to -1 + 2u_0 v_0 > 0 \to b > a$$
$$df_u + g_v > 0 \to d(b-a) > (b+a)^3 \ .$$

The sufficient condition is

$$df_u + g_v > 2\sqrt{\mathrm{Det}}\sqrt{d} \quad \text{or} \quad \boxed{\sqrt{d} > \frac{(b+a)^2}{(b-a)}\left(1 + \sqrt{\frac{2b}{b+a}}\right)}$$

Construct a stability diagram in a-b space