Exploring Turing Patterns

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August 12, 2018

Motivation

I recently came across a fascinating article[1] describing recent attempts to mathematically model how the brain creates visual hallucinations. That article, in turn, pointed me to the subject of so-called *Turing patterns* and, in particular, to Turing's paper on morphogenesis as possibly being due to the interplay between diffusion processes and the competition between activating and inhibiting chemicals.[2]

The potential applicability of Turing's hypothesis is mind-blowing. From how the patterns on the furs of animals form to how cells differentiate during the various phases of embryonic development and from how patterns form in sand dunes to how spiral arms form in galaxies, any time a process involves two competing entities (an activator and an inhibitor) spreading over space in a diffusive manner, the stage is set for Turing patterns to form.

From a purely mathematical point of view, Turing's paper is a particular application of a certain kind of partial differential equation. Mathematical physics has always been one of my favorite topics so I've decided to explore that same equation in a more systematic fashion than Turing's approach in that paper. I'm sure that nothing I'll be doing will be new but working through problems like this is fun, at least for me.

Turing patterns

The essence of Turing's insight is as follows. Imagine that the behaviour of a group of cells (for example, the skin cells of an animal such as a zebra or a giraffe) is determined by the concentrations of two kinds of chemicals, an activator and an inhinitor. For instance, if a

[1] *A Math Theory for Why People Hallucinate*,
https://www.quantamagazine.org/a-math-theory-for-why-people-hallucinate-20180730/

[2] *The Chemical Basis of Morphogenesis*,
http://www.dna.caltech.edu/courses/cs191/paperscs191/turing.pdf

particular kind of skin cell is exposed to a higher concentration of the activating chemical than of the inhibiting chemical, it will secrete a pigmenting chemical. Now, if the activating and inhibiting chemicals are spatially distributed over the animal's skin in a uniform manner then the animal's fur will have a uniform color. These chemicals, however, also diffuse and — crucially — can do so at different diffusion rates. If the inhibitor diffuses more quickly than the activator then it's possible for the two chemicals to achieve a steady-state *non-uniform* distribution thereby causing skin coloration patterns.

The example outlined above is specific to skin coloration in animals but the underlying process is much more general than that, requiring simply that two competing processes diffuse at different rates through the system under consideration.

Diffusion

The idea of diffusion is very simple. A quantity of some kind (a chemical substance, heat, information, etc) changes its concentration at a given point in space depending on its concentration at nearby points in such a manner that it flows from regions of high concentration to regions of low concentration. Diffusion is a kind of *transport phenomenon* characterized by the fact that the transport is due to a random process. For instance, the primary transport mechanism in the diffusion of gases is the random motion of their molecules.

Since the quantity being diffused is typically neither created nor destroyed, but only propagates from one point to another in space, it must satisfy the *continuity equation*,

$$\nabla \cdot \mathbf{j} + \frac{\partial q}{\partial t} = 0\,,$$

where q is the density of the quantity being diffused (its amount per unit of volume) and $\mathbf{j}$ is its current density (the amount per second that crosses a surface of unit area, oriented in a given direction). Both q and $\mathbf{j}$ change from point to point in space, and from moment to moment in time, and it's the continuity equation's job to tie together their variations in space and time. It is the local statement of the conservation of the quantity in question and corresponds to the idea that the only manner by which its concentration inside a closed surface changes is through the quantity crossing the surface's boundary.

On the other hand, it's typical of diffusion processes that the current density points in a direction *opposite* to the gradient of the density of the quantity being diffused,

$$\mathbf{j} = -\,d\,\nabla q\,,$$

where d, the *diffusion constant*, is a positive constant depending on the properties of the quantity being diffused and of the medium through which it's diffusing. In more complicated situations, it's actually not a single constant but a rank-2 tensor, and may even depend on position and/or time. In any case, this relation makes sense since the flow is from higher to lower concentrations, hence opposite to an increasing concentration gradient. Combining the two results above gives rise to the *diffusion equation*,

$$\frac{\partial q}{\partial t} = d\,\nabla^2 q\,.$$

Chemical reactions

Ignoring diffusion and other processes for the moment, the concentrations of N chemical substances reacting with one another can be described by a set of coupled equations of the form

$$\frac{\partial q_i}{\partial t} = f_i(q_1, q_2, \ldots, q_N)\,, \qquad 1 \le i \le N\,,$$

where the f_i are functions describing the details of the reactions involving the chemicals whose concentrations are represented by q_i. Note that these are completely local in space, *i.e.*, the increase or decrease in concentration at a given point in space is due entirely to the current concentrations at that point and does not depend on the concentrations at any other points, near or far.

Although these equations describe the time evolution of the concentrations of the various substances, in practice we're more interested in a steady-state solution, *i.e.*, a solution that does not change with time. If the set $\bar{q}_i{}^{(0)}(\mathbf{r})$ forms such a steady-state solution then

$$\frac{\partial \bar{q}_i{}^{(0)}}{\partial t} = f_i(\bar{q}_1^{(0)}, \bar{q}_2^{(0)}, \ldots, \bar{q}_N^{(0)}) \equiv 0\,, \qquad 1 \le i \le N\,.$$

The stability of chemical reactions in the presence of diffusion

We now combine both processes and write, for N substances reacting with each other as well as diffusing,

$$\boxed{\frac{\partial q_i}{\partial t} = d_i\,\nabla^2 q_i + f_i(q_1, q_2, \ldots, q_N)\,, \qquad 1 \le i \le N\,.}$$

We'd like to solve this set of equations with some prescribed set of initial conditions $q_i(t=0)$ and examine whether those solutions are stable. Of course, however, they cannot be solved without specifying the f_i functions.

The Linearised Equations

Conceptually, the effect of the diffusion terms $d_i\,\nabla^2 q_i$ is to decrease the local concentrations by "leaking" them into neighboring points in space. However, if the reaction terms f_i, which work as sources, are large enough to over-compensate for the diffusive loss then the local concentrations increase in time. This leads to an unstable solution where the concentrations grow exponentially large. On the other hand, if the source terms can't keep up with the diffusion, the local concentrations will decrease in time, eventually exhausting themselves. There is also the possibility that the two processes balance each other, the source terms providing just enough concentration to compensate for the diffusion. In that case we have a steady-state solution. Now, all three possibilities can happen at different points in space and differently for different reagents, so we can see how spatial patterns of high or low concentrations can happen. If these are time-independent, then we have steady-state Turing-like patterns.

We can find out what conditions give rise to unstable solutions by looking at the evolution of small deviations from a given state. If these small deviations already grow unbounded then the situation is already unstable.

So, imagine expanding $q_i(\mathbf{r},t)$ around some initial state $q_i^{(0)}(\mathbf{r},t)$. Defining $\xi_i = q_i - q_i^{(0)}$, we have

$$\begin{aligned} f_i(\{q\}) &= f_i(\{q^{(0)}\}) + \sum_j \frac{\partial f_i}{\partial q_j}\Big|_{\{q^{(0)}\}} (q_j - q_j^{(0)}) + \cdots \\ &= f_i^{(0)}(\mathbf{r},t) + \sum_j f_{ij}(\mathbf{r},t)\,\xi_j + \cdots \end{aligned}$$

where higher-order powers of ξ_j have been neglected. Note that the $f_i^{(0)}(\mathbf{r},t)$ and $f_{ij}(\mathbf{r},t)$ terms are known functions, since the initial states $q_i^{(0)}(\mathbf{r},t)$ are specified functions. Thus, in the presence of diffusion, the first-order deviations from the initial state must satisfy the equations

$$\frac{\partial \xi_i}{\partial t} + \frac{\partial q_i^{(0)}}{\partial t} = d_i\,\nabla^2 \xi_i + d_i\,\nabla^2 q_i^{(0)} + \sum_j f_{ij}\,\xi_j\,.$$

Now, *if* the initial state is time-independent, then $\dfrac{\partial q_i^{(0)}}{\partial t}$ vanishes identically, and we find

$$\frac{\partial \xi_i}{\partial t} = d_i\,\nabla^2 \xi_i + d_i\,\nabla^2 q_i^{(0)}(\mathbf{r}) + \sum_j f_{ij}(\mathbf{r})\,\xi_j\,.$$

Moreover, if the initial state is *also* homogeneous, then all the $d_i\,\nabla^2 q_i^{(0)}(\mathbf{r})$ terms also vanish identically and the $f_{ij}(\mathbf{r})$ coefficients turn into constants, and we're left with

$$\frac{\partial \xi_i}{\partial t} = d_i\,\nabla^2 \xi_i + \sum_j f_{ij}\,\xi_j\,, \qquad 1 \le i \le N\,.$$

It is convenient to rewrite the equations above in a more compact fashion. Defining a colum vector u of ξ_i functions, a matrix F of f_{ij} constants, and a diagonal matrix D of diffusion constants by

$$u = \begin{pmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_N \end{pmatrix}, \quad F = \begin{pmatrix} f_{11} & f_{12} & \cdots & f_{1N} \\ f_{21} & f_{22} & \cdots & f_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ f_{N1} & f_{N2} & \cdots & f_{NN} \end{pmatrix}, \quad \text{and} \quad D = \begin{pmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_N \end{pmatrix},$$

then the set of equations can be written more succintly as

$$\boxed{\frac{\partial u}{\partial t} = D\,\nabla^2 u + F u}\,.$$

To be absolutely clear, this is an equation for N components $(u_1, u_2, \ldots, u_N)$ in a space of any number of dimensions, and we're interested in solutions where the initial deviations are seeded by some known function, $u(t=0) = u^{(0)}(\mathbf{r})$. Note that $u^{(0)}$ is an N-component vector field.

The General Solution

If we Fourier-decompose $u(\mathbf{r}, t)$ by introducing the as-yet unknown function $u_{\mathbf{k}}(t)$ through

$$u(\mathbf{r}, t) = \int \frac{d\mathbf{k}}{(2\pi)^{n/2}}\; u_{\mathbf{k}}(t)\, \exp(i\,\mathbf{k}\cdot\mathbf{r})\,,$$

where n is the number of spatial dimensions we're working with, then $u_{\mathbf{k}}(t)$ must satisfy the equation

$$\frac{\partial u_{\mathbf{k}}}{\partial t} = -\,(k^2 D - F)\,u_{\mathbf{k}}\,.$$

This is trivially solvable, with the solution

$$u_{\mathbf{k}}(t) = A_{\mathbf{k}}\, \exp(-\omega_{\mathbf{k}}\, t)\,,$$

where $A_{\mathbf{k}}$ is an arbitrary N-component constant column vector and $\omega_{\mathbf{k}}$ is an eigenvalue of the matrix $(k^2 D - F)$:

$$\boxed{\left|k^2 D - F - \omega_{\mathbf{k}}\, I_N\right| = 0\,.}$$

The general solution to the original equation is then

$$u(\mathbf{r},t) = \int \frac{d\mathbf{k}}{(2\pi)^{n/2}}\; A_{\mathbf{k}}\, \exp(i\,\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}\, t)\,.$$

With the prescribed initial solution $u(\mathbf{r}, t=0) = u^{(0)}(\mathbf{r})$, then

$$u^{(0)}(\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^{n/2}}\; A_{\mathbf{k}}\, \exp(i\,\mathbf{k}\cdot\mathbf{r})\,,$$

which lets us determine $A_{\mathbf{k}}$ by applying an inverse Fourier transform:

$$\int \frac{d\mathbf{r}}{(2\pi)^{n/2}}\; u^{(0)}(\mathbf{r})\, \exp(-i\,\mathbf{k}'\cdot\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^{n/2}}\; A_{\mathbf{k}} \int \frac{d\mathbf{r}}{(2\pi)^{n/2}}\; \exp\left[i\,(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}\right]\,.$$

Since

$$\int \frac{d\mathbf{r}}{(2\pi)^{n/2}}\; \exp\left[i\,(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}\right] = \delta(\mathbf{k}-\mathbf{k}')\,,$$

we get

$$A_{\mathbf{k}} = \int \frac{d\mathbf{r}'}{(2\pi)^{n/2}}\; u^{(0)}(\mathbf{r}')\, \exp(-i\,\mathbf{k}\cdot\mathbf{r}')\,.$$

Substituting it back into the general solution gives us,

$$\boxed{u(\mathbf{r},t) = \int \frac{d\mathbf{k}}{(2\pi)^{n/2}}\; \exp(-\omega_{\mathbf{k}}\, t) \int \frac{d\mathbf{r}'}{(2\pi)^{n/2}}\; u^{(0)}(\mathbf{r}')\, \exp\left[i\,\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')\right]}\,.$$

This is the solution to the problem at hand, for any number of spatial dimensions and any number of components, given an arbitrary initial condition. Of course, it's not very useful yet in the form written above. Moreover, one of the more subtle and difficult parts has to do with solving the eigenvalue problem mentioned above, to determine the allowed values of $\omega_{\mathbf{k}}$.

The One-Component Equation

To get a better feeling for what's involved in making use of the above solution, let's look at the 1-component scenario. We have a single function u and single diffusion and reaction constants, d and f, respectively. Then,

$$\frac{\partial u}{\partial t} = d\,\nabla^2 u + f u\,.$$

and the general solution obtained above gives

$$u(\mathbf{r},t) = \int \frac{d\mathbf{k}}{(2\pi)^{n/2}}\ \exp(-\omega_{\mathbf{k}}\,t) \int \frac{d\mathbf{r}'}{(2\pi)^{n/2}}\ u^{(0)}(\mathbf{r}')\ \exp\left[i\,\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')\right]\ ,$$

where $u^{(0)}(\mathbf{r})$ is now just one function and $\omega_{\mathbf{k}}$ is given by

$$\omega_{\mathbf{k}} = k^2 d - f\,.$$

We thus see that wave vectors $\mathbf{k}$ such that $k^2 > f/d$ result in a positive $\omega_{\mathbf{k}}$ which, in turn, cause the solution to decay exponentially with time, eventually reaching the asymptotic value of zero. On the other hand, if $k^2 < f/d$, then $\omega_{\mathbf{k}} < 0$ and the corresponding solution grows exponentially large, thereby being an unstable solution. To prevent this from happening for any wave vector, we must require f to be negative. But, then, because $k^2 > f/d$ for all wave vectors, the system has no "interesting" solutions. The only interesting solution happens when $f > 0$ and $k^2 = f/d$. In this case, $\omega_{\mathbf{k}} \equiv 0$ and we have a steady-state solution.

Now, if the system is contained in a fixed volume of characteristic length L then we can have standing waves for wave vectors whose magnitudes are such that $k\,L$ is an integer multiple of 2π, in which case $k = (2\pi\,m)\,/\,L$, where m is a positive integer.[3] This, combined with $\omega_{\mathbf{k}} = 0$, gives us

$$\frac{4\pi^2}{L^2}\,m^2 = \frac{f}{d}\,.$$

[3] Actually, things are a little more complicated than that since there's a strong dependence on the specific geometry involved. For example, in two spatial dimensions and for rectangular Euclidean surfaces with periodic boundary conditions in both directions, then $k_x = (2\pi\,m_x)/L_x$ and $k_y = (2\pi\,m_y)/L_y$ and there are *two* integers defining the allowed standing wave modes. Then, $k^2 = f/d$ implies

$$k^2 = k_x^2 + k_y^2 = 4\pi^2\left(\frac{m_x^2}{L_x^2} + \frac{m_y^2}{L_y^2}\right) = \frac{f}{d}$$

for the modes with $\omega_{\mathbf{k}} = 0$. For the sake of argument, I've chosen to ignore this detail since it doesn't affect the main conclusion of this section and only adds complexity to an already dense text.

In other words, for systems with $f > 0$ and a characteristic length L satisfying

$$L = 2\pi\, m \sqrt{\frac{d}{f}}\,, \quad m = 1, 2, 3, \ldots\,,$$

there are steady-state solutions with standing waves. To obtain these solutions in detail, we need to perform the integration in $\mathbf{k}$-space with a fixed magnitude of

$$k = \frac{2\pi\, m}{L} = \sqrt{\frac{f}{d}}\,.$$

That we can do as follows. The elements of volume in $\mathbf{k}$-space, in $n = 1, 2, 3$ dimensions, the cases of interest here, are given by

$$d\mathbf{k} = \begin{cases} dk\,, & \text{if } n = 1\,, \\ k\, dk\, d\varphi\,, & \text{if } n = 2\,, \\ k^2\, dk\, \sin\theta\, d\theta\, d\varphi\,, & \text{if } n = 3\,. \end{cases}$$

Thus, choosing an appropriate orientation for the coordinate axes in $\mathbf{k}$-space for each value of n, we find

- $n = 1$:
$$u(x) = \frac{1}{2\pi i} \int_0^L dx'\, \frac{u^{(0)}(x')}{(x - x')}\, \exp\left[i\, k(x - x')\right]\,.$$
- $n = 2$:
$$u(\mathbf{r}) = \frac{1}{2\pi} \int d\mathbf{r}'\, u^{(0)}(\mathbf{r}')\; k^2\, J_0(k\, |\mathbf{r} - \mathbf{r}'|)\,,$$
where $J_0(s)$ is the Bessel function of the first kind, of order zero.
- $n = 3$:
$$u(\mathbf{r}) = \frac{1}{2\pi} \int d\mathbf{r}'\, u^{(0)}(\mathbf{r}')\; \frac{k^2 \sin\left(k\, |\mathbf{r} - \mathbf{r}'|\right)}{|\mathbf{r} - \mathbf{r}'|}\,.$$

Note that, in all 3 cases,[4]

$$k = \frac{2\pi\, m}{L} = \sqrt{\frac{f}{d}}\,.$$

[4]More accurately,

$$k = 2\pi \sqrt{\frac{m_x^2}{L_x^2} + \frac{m_y^2}{L_y^2}} = \sqrt{\frac{f}{d}}$$

as per the previous footnote.

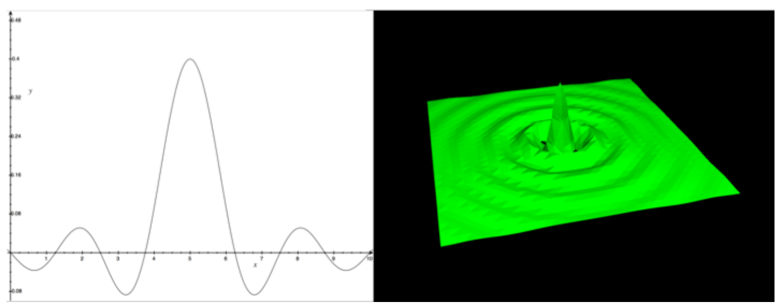
No more progress can be made without selecting the initial condition $u^{(0)}(\mathbf{r})$. For instance, suppose that the initial condition is a "lump" concentrated at $\mathbf{r} = \mathbf{r}_0$, *i.e.*, the delta function $\delta(\mathbf{r} - \mathbf{r}_0)$. Then:

- $n = 1$:
$$u(x) = \frac{k}{2\pi} \frac{\sin\left[\, k\,(x - x_0)\,\right]}{k\,(x - x_0)}\,.$$

- $n = 2$:
$$u(\mathbf{r}) = \frac{k^2}{2\pi}\; J_0(k\,|\mathbf{r} - \mathbf{r}_0|)\,.$$

- $n = 3$:
$$u(\mathbf{r}) = \frac{k^3}{2\pi}\, \frac{\sin\left(k\,|\mathbf{r} - \mathbf{r}_0|\right)}{k|\mathbf{r} - \mathbf{r}_0|}\,.$$

Here are plots of the solutions above, for 1 and 2 dimensions, for the $m = 4$ standing wave modes. As one can see, these solutions aren't all that interesting in regards to Turing patterns. For more interesting patterns to appear, we need more components, *i.e.*, more reagents feeding each other.



The Two-Component Equation

Much of what was obtained in the previous sections is still valid for two components. In particular, all four boxed results still apply. The key difference is that, with two or more components, the equations involve matrices and their eigenvalue problems. In fact, we saw previously that solutions of the form

$$u_{\mathbf{k}}(\mathbf{r}, t) = \exp(i\,\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}\,t)$$

are possible, provided that $\omega_{\mathbf{k}}$ is an eigenvalue of the matrix $M_{\mathbf{k}} = (k^2 D - F)$. With $N = 2$ components, this eigenvalue problem reduces to solving the characteristic equation

$$\left|k^2 D - F\right| = \begin{vmatrix} d_1 k^2 - f_{11} - \omega_{\mathbf{k}} & -f_{12} \\ -f_{21} & d_2 k^2 - f_{22} - \omega_{\mathbf{k}} \end{vmatrix} = \omega_{\mathbf{k}}^2 - \mathrm{Tr}(M_{\mathbf{k}})\,\omega_{\mathbf{k}} + |M_{\mathbf{k}}| = 0\,,$$

whose solution is

$$\boxed{\omega_{\mathbf{k}} = \frac{\mathrm{Tr}(M_{\mathbf{k}})}{2} \pm \sqrt{\left[\frac{\mathrm{Tr}(M_{\mathbf{k}})}{2}\right]^2 - |M_{\mathbf{k}}|}\,,}$$

where $\mathrm{Tr}(M_{\mathbf{k}})$ is the *trace* of $M_{\mathbf{k}}$, that is, the sum of its diagonal elements,

$$\boxed{\begin{aligned} \mathrm{Tr}(M_{\mathbf{k}}) \;&=\; \mathrm{Tr}(k^2 D - F) \;=\; (d_1 + d_2)\, k^2 - (f_{11} + f_{22}) \qquad \text{and} \\ |M_{\mathbf{k}}| \;&=\; \quad |k^2 D - F| \;=\; d_1\, d_2\, k^4 - (d_1\, f_{22} + d_2\, f_{11})\, k^2 + (f_{11}\, f_{22} - f_{12}\, f_{21})\,. \end{aligned}}$$

Detailed analysis

We've arrived in the previous section to the result that small deviations $u(\mathbf{r}, t)$ from the non-diffusive homogeneous steady-state solution are, in the presence of diffusion, linear combinations of plane-wave solutions of the form

$$u_{\mathbf{k}}(\mathbf{r}, t) = \exp(i\, \mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}}\, t)\,,$$

with the *dispersion relation*

$$\omega_{\mathbf{k}} = \frac{(d_1 + d_2)\, k^2 - (f_{11} + f_{22})}{2} \pm \sqrt{\frac{[(d_1 - d_2)\, k^2 - (f_{11} - f_{22})]^2}{4} + f_{12}\, f_{21}}\,.$$

Note that a plane-wave solution with $k^2 = 0$ is a possible contribution. Now, when $k^2 = 0$, the D-dependent term in

$$\frac{\partial u_{\mathbf{k}}}{\partial t} = (F - k^2 D)\, u_{\mathbf{k}}$$

drops out and diffusion does not contribute to the time evolution of that solution. In the absence of diffusion, however, our solution is the homogeneous steady-state one so we need to require the small deviations to vanish altogether, or at least die out exponentially, so the homogeneous steady-state solution remains so, and stable, when $k^2 = 0$.[5] We can use

[5] Physically, the interpretation of $k^2 = 0$ is the following. The magnitude of $\mathbf{k}$, $k = |\mathbf{k}|$, is the inverse (up to a factor of 2π) of the wavelength of the particular plane wave associated with $\mathbf{k}$. When k is non-zero, that wavelength provides the length scale at which we can expect the solution to vary in space. However, our steady-state solution in the absence of diffusion is homogeneous, meaning that its variation in space has a very large scale (formally, infinite), therefore having a very large (formally, infinite) wavelength. An infinite wavelength corresponds to a $\mathbf{k}$ vector with zero magnitude, hence $k^2 = 0$. Thus, requiring the small-deviations solution in the absence of diffusion to fall back to the homogeneous steady-state one corresponds to requiring them to vanish altogether, or at least die out exponentially, for $k^2 = 0$.

the $\exp(-\omega_{\mathbf{k}}\, t)$ factor in the solutions to make the small deviations die out exponentially by requiring $\omega_{\mathbf{k}}$ to be real and *positive* when $k^2 = 0$. Now,

$$\omega_{\mathbf{k}=\mathbf{0}} = -\frac{\mathrm{Tr}(F)}{2} \pm \sqrt{\left[\frac{\mathrm{Tr}(F)}{2}\right]^2 - |F|}\ .$$

This is real when $\big[\mathrm{Tr}(F)\big]^2 \geq 4|F|$ and, in that case, always positive if $\mathrm{Tr}(F) < 0$ and $|F| \geq 0$. Thus, to guarantee the stability of the homogeneous steady-state solution, we must require the following three conditions on the coefficients of F:

$$\boxed{\begin{array}{rcll} \mathrm{Tr}(F) < 0 & \Rightarrow & f_{11} + f_{22} < 0\,, & \\ |F| \geq 0 & \Rightarrow & f_{11}\, f_{22} \geq f_{12}\, f_{21}\,, & \text{and} \\ \big[\mathrm{Tr}(F)\big]^2 \geq 4|F| & \Rightarrow & (f_{11} - f_{22})^2 \geq -4\, f_{12}\, f_{21}\,. & \end{array}}$$

Note that the last condition is always satisfied if f_{12} and f_{21} have the same sign (both positive or both negative), or if at least one of them vanishes.

Having looked at the contribution from $k^2 = 0$, we now ask if we should consider contributions with $k^2 < 0$. These would have imaginary wave vectors which, through the $\exp(i\,\mathbf{k}\cdot\mathbf{r})$ factor, would cause the small-deviation solutions to either grow exponentially large or decay exponentially, as the plane-waves they correspond to travel through the diffusing medium. Considering that actual physical systems are always finite in size, these contributions might actually be acceptable for certain combinations of the parameters. However, it's likely that exponentially increasing deviations would cease to be sufficiently small after they travel a few wavelengths in space so the linearised approximation that we've employed is likely to break down. Because of these considerations, we'll require k^2 to be non-negative.

We now proceed to examine solutions with $k^2 > 0$ and their impact on $\omega_{\mathbf{k}}$. Ultimately, for $k^2 > 0$, we want solutions where the real part of $\omega_{\mathbf{k}}$ vanishes. That's because $\omega_{\mathbf{k}}$ values with a non-vanishing real part will cause the small-deviation solutions to either grow exponentially large, or die out, as time passes, neither of which leads to persistent spatial patterns.

There are, thus, two cases to consider:

- $\omega_{\mathbf{k}}$ **vanishes identically**, in which case the small-deviation solutions are non-homogeneous but time-independent: From the characteristic determinant shown previously, we see that a necessary condition for $\omega_{\mathbf{k}}$ to vanish is $|M_{\mathbf{k}}| = 0$. However, in this case, there is a second solution, $\omega_{\mathbf{k}} = \mathrm{Tr}(M_{\mathbf{k}})$. In order for this second solution not to cause an instability that grows to overcome the solution with $\omega_{\mathbf{k}} = 0$, we need also to have $\mathrm{Tr}(M_{\mathbf{k}}) > 0$ (so the $\exp(-\omega_{\mathbf{k}}\, t)$ factor causes the offending solution to die out). Thus, in order for $\omega_{\mathbf{k}} = 0$ to result in a stable, persistent, non-homogeneous, and time-independent solution we need

$$\mathrm{Tr}(M_{\mathbf{k}}) > 0 \quad \Rightarrow \quad (d_1 + d_2)\, k^2 - (f_{11} + f_{22}) > 0 \qquad \text{and}$$

$$|M_{\mathbf{k}}| = 0 \quad \Rightarrow \quad d_1\, d_2\, k^4 - (d_1\, f_{22} + d_2\, f_{11})\, k^2 + (f_{11}\, f_{22} - f_{12}\, f_{21}) = 0\,.$$

The first condition is automatically satisfied since the diffusion coefficients are positive and $f_{11} + f_{22}$ is assumed negative, as per the discussion of solutions for $k^2 = 0$. The second condition gives us potentially allowed values for k^2:

$$\boxed{{k^2}_{\pm} = \frac{(d_1\, f_{22} + d_2\, f_{11})}{2\, d_1\, d_2} \pm \sqrt{\left[\frac{(d_1\, f_{22} + d_2\, f_{11})}{2\, d_1\, d_2}\right]^2 - \frac{(f_{11}\, f_{22} - f_{12}\, f_{21})}{d_1\, d_2}}\,.}$$

We still need these to be real and positive values, so we must also have:

$$\boxed{\begin{aligned} d_1\, f_{22} + d_2\, f_{11} &> 0\,, \\ f_{11}\, f_{22} &\geq f_{12}\, f_{21}\,, \qquad \text{and} \\ (d_1\, f_{22} + d_2\, f_{11})^2 &\geq 4\, d_1\, d_2\, (f_{11}\, f_{22} - f_{12}\, f_{21})\,. \end{aligned}}$$

- $\omega_{\mathbf{k}}$ **is purely imaginary**, in which case the small-deviation solutions would be traveling plane waves. This situation cannot happen, however, because we're requiring $f_{11} + f_{22} < 0$ and a purely imaginary $\omega_{\mathbf{k}}$ requires $\mathrm{Tr}(M_{\mathbf{k}}) = 0$, leading to

$$k^2 = \frac{f_{11} + f_{22}}{d_1 + d_2}$$

  and, thus, a negative k^2.

Summary of the stability analysis

We have concluded that the only stable solutions are those with $k^2 = 0$, in which case

$$\omega_{\mathbf{k}=\mathbf{0}} = -\frac{(f_{11} + f_{22})}{2} \pm \sqrt{\left[\frac{(f_{11} - f_{22})}{2}\right]^2 + f_{12}\, f_{21}} > 0\,,$$

and those with

$$k^2 = \frac{(d_1\, f_{22} + d_2\, f_{11})}{2\, d_1\, d_2} \pm \sqrt{\left[\frac{(d_1\, f_{22} + d_2\, f_{11})}{2\, d_1\, d_2}\right]^2 - \frac{(f_{11}\, f_{22} - f_{12}\, f_{21})}{d_1\, d_2}}\,,$$

in which case $\omega_{\mathbf{k}} = 0$. Moreover, in order for these to be, in fact, stable solutions, the following conditions must be set on the various parameters:

1. $f_{11} + f_{22} < 0$
2. $(f_{11} - f_{22})^2 \geq -4\, f_{12}\, f_{21}$
3. $f_{11}\, f_{22} - f_{12}\, f_{21} \geq 0$
4. $d_1\, f_{22} + d_2\, f_{11} > 0$
5. $(d_1\, f_{22} + d_2\, f_{11})^2 \geq 4\, d_1\, d_2\, (f_{11}\, f_{22} - f_{12}\, f_{21})$

More on the conditions over the reaction and diffusion parameters

The conditions on the various parameters, summarised at the end of the previous section, can be made clearer by establishing certain proportionalities between those parameters. Starting with f_{11} and f_{22}, let α be defined by $\boxed{f_{22} = \; -\,\alpha\, f_{11}}$ and let's assume $\boxed{f_{11} > 0}$. Then:

1. $f_{11} + f_{22} < 0$ implies $\boxed{\alpha > 1}$;
2. $(f_{11} - f_{22})^2 \geq -4\, f_{12}\, f_{21}$ implies $\boxed{f_{12}\, f_{21} \geq \; -\, \frac{(\alpha+1)^2}{4}\, f_{11}^2}$;
3. $f_{11}\, f_{22} - f_{12}\, f_{21} \geq 0$ implies $\boxed{f_{12}\, f_{21} \leq \; -\,\alpha\, f_{11}^2}$;
4. $d_1\, f_{22} + d_2\, f_{11} > 0$ implies $d_2 > \alpha\, d_1$ so let β be defined by $\boxed{d_2 = \alpha\, \beta\, d_1}$. Then, since $\alpha > 1$ and $\boxed{d_1 > 0}$, it follows that $\boxed{\beta > 1}$;
5. $(d_1\, f_{22} + d_2\, f_{11})^2 \geq 4\, d_1\, d_2\, (f_{11}\, f_{22} - f_{12}\, f_{21})$ implies $\boxed{f_{12}\, f_{21} \geq \; -\, \frac{\alpha}{\beta}\, \frac{(\beta+1)^2}{4}\, f_{11}^2}$.

The three conditions on $f_{12}\, f_{21}$ can be combined into:

$$\boxed{\alpha \;\leq\; -\,\frac{f_{12}\, f_{21}}{f_{11}^2} \;\leq\; \frac{1}{4} \min\left\{ (\alpha+1)^2 \,,\, \frac{\alpha}{\beta}\, (\beta+1)^2 \right\}.}$$

It's not difficult to show that

$$\min\left\{ (\alpha+1)^2 \,,\, \frac{\alpha}{\beta}\, (\beta+1)^2 \right\} = \begin{cases} (\alpha+1)^2 \,, & \text{if } \alpha \leq \beta \,, \\ \frac{\alpha}{\beta}\, (\beta+1)^2 \,, & \text{if } \alpha > \beta \,. \end{cases} \,,$$

and that, in either case, $4\,\alpha$ is no larger than that minimum. In other words, it's always possible to find a value of $f_{12}\, f_{21}$ that satisfies the condition above.

So... what's the solution?

We've seen that the general solution to the problem we're trying to solve is a superposition of plane-waves of the form

$$u_{\mathbf{k}}(\mathbf{r},t) = \exp(i\,\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}\,t)\,.$$

In other words, the general solution for small deviations $u(\mathbf{r},t)$ from the steady-state solution is given by (the real part of)

$$u(\mathbf{r},t) = \int \frac{d\mathbf{k}}{(2\pi)^{n/2}}\,\bar{u}_{\mathbf{k}}\,\exp(i\,\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}\,t)\,,$$

where n is the number of spatial dimensions under consideration and the factor $(2\pi)^{n/2}$ is added for convenience. The initial condition is some given 2-component vector field $u_0(\mathbf{r})$, so

$$u(\mathbf{r},t=0) = \int \frac{d\mathbf{k}}{(2\pi)^{n/2}}\,\bar{u}_{\mathbf{k}}\,\exp(i\,\mathbf{k}\cdot\mathbf{r}) = u_0(\mathbf{r})\,.$$

This equation shows that $u_0(\mathbf{r})$ and $\bar{u}_{\mathbf{k}}$ form a Fourier-transform pair, meaning that

$$\bar{u}_{\mathbf{k}} = \int \frac{d\mathbf{r}}{(2\pi)^{n/2}}\,u_0(\mathbf{r})\,\exp(-i\,\mathbf{k}\cdot\mathbf{r})\,.$$

Changing the integration variable from $\mathbf{r}$ to $\mathbf{r}'$ and plugging this back into the general solution gives us

$$\boxed{u(\mathbf{r},t) = \int \frac{d\mathbf{k}}{(2\pi)^{n/2}} \int \frac{d\mathbf{r}'}{(2\pi)^{n/2}}\,u_0(\mathbf{r}')\,\exp\Big[\,i\,\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}') - \omega_{\mathbf{k}}\,t\,\Big]}\,.$$

In two or more spatial dimensions, a vector has a direction as well as a magnitude. For instance, in $n=2$ dimensions, using polar coordinates in $\mathbf{k}$-space with its x-axis along $(\mathbf{r}-\mathbf{r}')$, $d\mathbf{k} = k\,dk\,d\theta$, and we have

$$\begin{aligned}
u(\mathbf{r},t) &= \int \frac{k\,dk\,d\theta}{2\pi} \int \frac{d\mathbf{r}'}{2\pi}\,u_0(\mathbf{r}')\,\exp\Big(i\,k\,|\mathbf{r}-\mathbf{r}'|\,\cos\theta - \omega_{\mathbf{k}}\,t\Big) \\
&= \int \frac{d\mathbf{r}'}{2\pi}\,u_0(\mathbf{r}') \int \frac{dk^2}{4\pi}\,\exp(-\omega_{\mathbf{k}}\,t) \int_0^{2\pi} d\theta\,\exp\Big(i\,k\,|\mathbf{r}-\mathbf{r}'|\,\cos\theta\Big) \\
&= \int \frac{d\mathbf{r}'}{4\pi}\,u_0(\mathbf{r}') \int dk^2\,J_0(k\,|\mathbf{r}-\mathbf{r}'|)\,\exp(-\omega_{\mathbf{k}}\,t)\,,
\end{aligned}$$

or

$$\boxed{u(\mathbf{r},t) = \int \frac{d\mathbf{r}'}{4\pi}\,u_0(\mathbf{r}') \int dk^2\,J_0(k\,|\mathbf{r}-\mathbf{r}'|)\,\exp(-\omega_{\mathbf{k}}\,t)}\,,$$

where $J_0(s)$ is the Bessel function of the 1st kind, of order 0. The above is the general solution, in two dimensions, for any initial distribution $u_0(\mathbf{r})$ of deviations from the diffusion-free steady-state solution.

Suppose, for example, that the initial distribution of deviations is concentrated at one point, $\mathbf{r}_0$. In other words, suppose that $u_0(\mathbf{r}) = 4\pi\,\delta(\mathbf{r}-\mathbf{r}_0)$ (the 4π factor is for convenience). The solution then becomes

$$u(\mathbf{r}, t) = \int dk^2\, J_0(k\,|\mathbf{r} - \mathbf{r}_0|)\, \exp(-\omega_{\mathbf{k}}\, t)\,.$$

What this equation says is that an initial "lump" propagates in space as a Bessel function but decays exponentially in time (if $\omega_{\mathbf{k}}$ is positive for the wave-vector in question).

However, the only stable, persistent and non-homogeneous solutions are time-independent (*i.e.*, have $\omega_{\mathbf{k}} = 0$), with $k^2 = k_+^2$ or $k^2 = k_-^2$, where

$$k^2{}_\pm = \frac{(d_1\, f_{22} + d_2\, f_{11})}{2\, d_1\, d_2} \pm \sqrt{\left[\frac{(d_1\, f_{22} + d_2\, f_{11})}{2\, d_1\, d_2}\right]^2 - \frac{(f_{11}\, f_{22} - f_{12}\, f_{21})}{d_1\, d_2}}\,.$$

Thus, for a single lump initially concentrated at $\mathbf{r}_0$, the resulting stable, persistent, non-homogeneous and time-independent pattern will have the form

$$u(\mathbf{r}) = A_+\, J_0(k_+\,|\mathbf{r} - \mathbf{r}_0|) + A_-\, J_0(k_-\,|\mathbf{r} - \mathbf{r}_0|)\,,$$

where A_+ and A_- are arbitrary constants. Note that $|\mathbf{r} - \mathbf{r}_0| = \sqrt{(x - x_0)^2 + (y - y_0)^2}\,$.

■