PHY256/PHY411 Lecture notes: Reaction-Diffusion Equations and Pattern Formation

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1 Reaction-Diffusion equations

Alan Turing found mathematical models that would produce spatial patterns from arbitrary initial states. These models were based on coupled chemical reactions but have since been applied in numerous fields.

1.0.1 The diffusion or heat equation

Let u be a concentration of something, e.g., numbers of molecules per unit volume.

The gradient of the concentration of u is $\boldsymbol{\nabla} u$. The rate of flow $\mathbf{F}$ or flux of u should depend on the gradient $\mathbf{F} = -D\boldsymbol{\nabla} u$. The rate of change of u then depends on the divergence of the flux or

$$\frac{\partial u}{\partial t} = -\boldsymbol{\nabla} \cdot \mathbf{F}.$$

We expect there to be change in the local quantity of u only if there is variation in the gradient of the flux. If the coefficient D is independent of position then we find

$$\frac{\partial u}{\partial t} = D\nabla^2 u$$

which is known as the diffusion equation or if we replace u with temperature T, it is called the heat equation.

1.0.2 Reaction Diffusion equations

Consider u and v to be concentrations of two chemicals. This means $u \geq 0$ and $v \geq 0$. The chemicals can diffuse through space and they can react with one another and with other reagents.

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u + f_u(u, v) \tag{1}$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + f_v(u, v). \tag{2}$$

Here D_u, D_v are the diffusion coefficients for u and v respectively. The functions $f_u(u, v)$ and $f_v(u, v)$ are the local reaction rates. In two dimensions $u(x, y, t)$ and $v(x, y, t)$ and the Laplacian operator $\Delta = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$.

1.1 The Brusselator model

The Brusselator model (developed by a group in Brussels) has reactions

$$\begin{aligned} \alpha &\to u \\ \beta + u &\to v \\ 2u + v &\to 3u \\ u &\to E \end{aligned}$$

where the concentrations of the reagents $\alpha, \beta, E \geq 0$ are kept constant. The reactions together give

$$f_u(u, v) = \alpha - (\beta + 1)u + u^2 v \tag{3}$$

$$f_v(u, v) = \beta u - u^2 v. \tag{4}$$

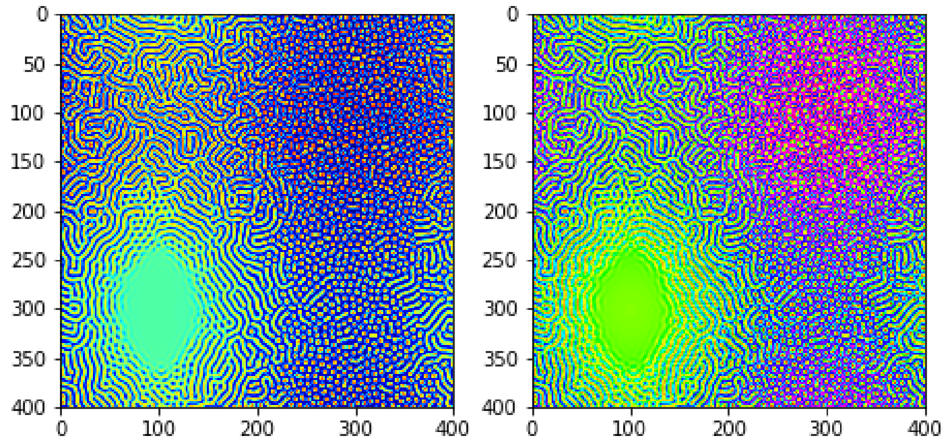

Figure 1: Patterns formed with the Brusselator model. u is on the left and v on the right. The grid has a sinusoidal variation in α (horizontally on the grid) and β (vertically on the grid). The mean values are $\alpha_m = 5$ and $\beta_m = 9$ with amplitudes of variation 1 and 1. Diffusion coefficients are $D_u = 2, D_v = 22$, the grid is $n = 400$ grid points and square and $\Delta x = 1, \Delta t = 0.0025$. The axes are x, y. Boundary conditions are periodic. The patterns grow and then become fixed.

Here α is a feeding rate for u. The parameter β is a kill rate for u that converts u to v. The uv^2 term is a reaction term, producing u at the expense of v.

Allowing u, v to also diffuse

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u + \alpha - (\beta + 1)u + u^2 v \tag{5}$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + \beta u - u^2 v. \tag{6}$$

This set of coupled equations displays a variety of phenomena, including growth of patterns (see Figure 1) and long lived oscillating behavior (see Figure 3).

1.1.1 The steady state of the Brusselator model

We consider the reaction alone. What is the steady state solution? The steady state solution satisfies

$$f_u(u, v) = \alpha - (\beta + 1)u + u^2 v = 0$$
$$f_v(u, v) = \beta u - u^2 v = 0$$

The second equation gives $\beta = uv$ and this in the first equation gives $\alpha = u$ and consequently $v = \beta/\alpha$. The steady state solution is

$$\begin{aligned} u_0 &= \alpha \\ v_0 &= \frac{\beta}{\alpha}. \end{aligned} \tag{7}$$

We can consider trajectories on the u, v plane. The steady state solution is a fixed point.

1.2 Wavelengths of the patterns that grow

To try to understand which types of patterns grow we look at the stability of perturbations near the steady state solution. Using linearized equations we estimate the growth rate as a function of wavevector or wavelength.

1.2.1 Linear analysis near the steady state solution for the Brusselator model

We assume a solution that is near the steady state solution.

$$\begin{aligned} u(x, y, t) &= u_0 + u_1(x, y, t) \\ v(x, y, t) &= v_0 + v_1(x, y, t), \end{aligned} \tag{8}$$

where the steady state solution satisfies

$$\begin{aligned} f_u(u_0, v_0) &= 0 \\ f_v(u_0, v_0) &= 0. \end{aligned}$$

We expand the equations of motion to first order in u_1, v_1, assuming that they are small.

We write down the equation of motion again (equation 6)

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u + \alpha - (\beta + 1)u + u^2 v \tag{9}$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + \beta u - u^2 v. \tag{10}$$

Here is how to compute the non-linear terms

$$\begin{aligned} u^2 v &= (u_0 + u_1)^2 (v_0 + v_1) \\ &= (u_0^2 + 2u_0 u_1 + u_1^2)(v_0 + v_1) \\ &= u_0^2 v_0 + 2u_0 u_1 v_0 + u_1^2 v_0 + u_0^2 v_1 + 2u_0 u_1 v_1 + u_1^2 v_1 \\ &= u_0^2 v_0 + 2u_0 v_0 v_1 + u_0^2 v_1 + ... \end{aligned}$$

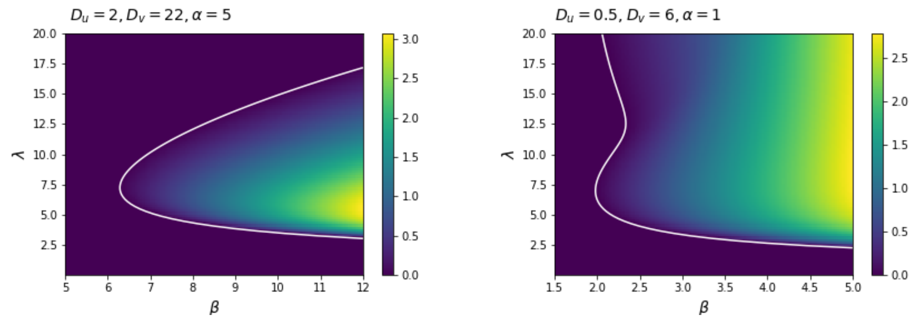

Figure 2: The real part $\gamma_+(k)$ giving the growth rate of perturbations for the Brusselator model. The left axis shows the wavelength $\lambda = 2\pi/k$. The diffusion coefficients and α are fixed and equation 14 used to compute the growth rate as a function of wave-vector k and parameter β. The parameter α and diffusion coefficients are printed on the top of the figures. Negative portions of the images are not shown. The white lines show zero growth rate. If the diffusion coefficients are reduced, smaller wavelengths can become unstable.

The first order terms are $2u_0v_0v_1 + u_0^2v_1$.

We plug equations 8 into the equations of motion and only keep zeroth and first order terms

$$u_{0,t} + u_{1,t} = D_u(u_{0,xx} + u_{1,xx} + u_{0,yy} + u_{1,yy}) + \alpha - (\beta+1)(u_0 + u_1) + u_0^2v_0 + 2u_0v_0v_1 + u_0^2v_1$$
$$v_{0,t} + v_{1,t} = D_v(v_{0,xx} + v_{1,xx} + v_{0,yy} + v_{1,yy}) + \beta(u_0 + u_1) - u_0^2v_0 - 2u_0v_0v_1 + u_0^2v_1.$$

The steady state solution has $u_{0,xx} = 0$, $u_{0,yy} = 0$, $u_{0,t} = 0$ and $v_{0,xx} = 0$, $v_{0,yy} = 0$, $v_{0,xx} = 0$. Deleting those terms we get

$$u_{1,t} = D_u(u_{1,xx} + u_{1,yy}) - (\beta+1)u_1 + 2u_0v_0v_1 + u_0^2v_1 + \alpha - (\beta+1)u_0 + u_0^2v_0$$
$$v_{1,t} = D_v(v_{1,xx} + v_{1,yy}) + \beta u_1 - u_0^2v_0 - 2u_0v_0v_1 + u_0^2v_1 + \beta u_0 - u_0^2v_0.$$

The terms that are zeroth order now drop out precisely because they involve the steady state solution. We delete the zero-th order terms. To first order in u_1, v_1 and in two dimensions the equations of motion for the Brusselator model are

$$u_{1,t} = D_u(u_{1,xx} + u_{1,yy}) - (\beta+1)u_1 + u_0^2v_1 + 2u_0v_0u_1$$
$$v_{1,t} = D_v(v_{1,xx} + v_{1,yy}) + \beta u_1 - u_0^2v_1 - 2u_0v_0u_1.$$

Using the steady state solution this becomes

$$u_{1,t} = D_u(u_{1,xx} + u_{1,yy}) + (\beta-1)u_1 + \alpha^2v_1$$
$$v_{1,t} = D_v(v_{1,xx} + v_{1,yy}) - \beta u_1 - \alpha^2v_1.$$

We adopt a trial solution in the form

$$u_1 = \tilde{u}_1 e^{\gamma t + ik_x x + ik_y y}$$
$$v_1 = \tilde{v}_1 e^{\gamma t + ik_x x + ik_y y}$$

giving

$$\left[\gamma + D_u(k_x^2 + k_y^2) - (\beta - 1)\right] \tilde{u}_1 = \alpha^2 \tilde{v}_1$$
$$\left[\gamma + D_v(k_x^2 + k_y^2) + \alpha^2\right] \tilde{v}_1 = -\beta \tilde{u}_1.$$

We combine these together to find

$$\left[\gamma + D_u(k_x^2 + k_y^2) - (\beta - 1)\right] \left[\gamma + D_v(k_x^2 + k_y^2) + \alpha^2\right] + \alpha^2 \beta = 0$$

This can be called the 'characteristic equation'.

The characteristic equation is a quadratic equation for γ that is a function of $k^2 = k_x^2 + k_y^2$ and parameters α, β. This characteristic equation can be written in the form

$$\gamma^2 + B(k)\gamma + C(k) = 0 \tag{11}$$

with coefficients

$$B(k) = (D_u + D_v)k^2 + \alpha^2 - \beta + 1 \tag{12}$$
$$C(k) = D_u D_v k^4 + D_u k^2 \alpha^2 + D_v k^2 (1 - \beta) + \alpha^2. \tag{13}$$

The quadratic formula

$$\gamma(k) = -\frac{B(k)}{2} \pm \frac{1}{2}\sqrt{B^2(k) - 4C(k)}. \tag{14}$$

If there are values of wave vector k giving solutions for γ that have a positive real part, these would correspond to perturbations that can grow exponentially quickly.

What wavevectors give a zero growth rate? These can be considered transition regions and they would satisfy $C(k) = 0$.

Because $B(k), C(k)$ are real functions, the larger of the two possible values for $\mathrm{Re}\gamma$

$$\mathrm{Re}\gamma_+(k) = \begin{cases} -\frac{B(k)}{2} + \frac{1}{2}\sqrt{B^2(k) - 4C(k)} & \text{if} \quad B^2(k) - 4C(k) \geq 0 \\ -\frac{B(k)}{2} & \quad\;\; B^2(k) - 4C(k) < 0 \end{cases} \tag{15}$$

The Brusselator model is specified by four parameters D_u, D_v, α, β, but growth rate γ_+ also depends on k. If you fix three of the parameters, say D_u, D_v, α, you can show on a two-d plot (the other two degrees of freedom β, k axes) the value of $\mathrm{Re}\gamma_+$. Where this is positive, you expect growth of structure with wavelength $2\pi/k$ and with growth rate given by $\mathrm{Re}\gamma_+$. See Figure 2 for some plots of $\mathrm{Re}\gamma_+$.

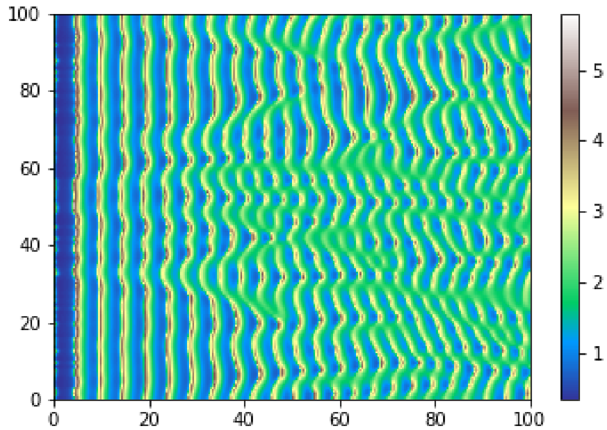

Figure 3: The Brusselator model in 1-dimension integrated with $D_u = 0.3, D_v = D_u/8$, $\alpha = 2$, $\beta = 5.4$, $\Delta x = 1$, $\Delta t = 0.005$. The horizontal axis is time, and the vertical axis is x. The boundary condition is periodic. This shows both development of spatial patterns and time dependent structures.

1.2.2 Linear analysis with a Jacobian

Using reaction functions to first order about the steady state solution

$$
\begin{aligned}
f_u(u_0 + u_1, v_0 + v_1) &= f_u(u_0, v_0) + \left.\frac{\partial f_u}{\partial u}\right|_{u_0, v_0} u_1 + \left.\frac{\partial f_u}{\partial v}\right|_{u_0, v_0} v_1 \\
f_v(u_0 + u_1, v_0 + v_1) &= f_v(u_0, v_0) + \left.\frac{\partial f_v}{\partial u}\right|_{u_0, v_0} u_1 + \left.\frac{\partial f_v}{\partial v}\right|_{u_0, v_0} v_1.
\end{aligned}
$$

Let $\mathbf{u} = (u, v)$ and $\mathbf{f}(\mathbf{u}) = (f_u(\mathbf{u}), f_v(\mathbf{u}))$. The steady state solution $\mathbf{u}_0$ satisfies $\mathbf{f}(\mathbf{u}_0) = 0$. Expanding about the steady state solution

$$
\mathbf{f}_u(\mathbf{u}_0 + \mathbf{u}_1) = \mathbf{f}_u(\mathbf{u}_0) + \left.\mathbf{Df}\right|_{\mathbf{u}_0} \mathbf{u}_1 + ...
$$

where $\mathbf{Df}$ is the Jacobian matrix. For the Brusselator model, the Jacobian matrix

$$
\begin{aligned}
\mathbf{Df} &= \begin{pmatrix} \frac{\partial f_u}{\partial u} & \frac{\partial f_u}{\partial v} \\ \frac{\partial f_v}{\partial u} & \frac{\partial f_v}{\partial v} \end{pmatrix} \\
&= \begin{pmatrix} -(\beta + 1) + 2uv & u^2 \\ \beta - 2uv & -u^2 \end{pmatrix}.
\end{aligned}
$$

Evaluated at the steady state solution or fixed point (equation 7) the Jacobian matrix

$$\mathbf{Df}\Big|_{\mathbf{u}_0} = \begin{pmatrix} \beta - 1 & \alpha^2 \\ -\beta & -\alpha^2 \end{pmatrix}. \tag{16}$$

The equation of motion in vector form

$$\frac{\partial \mathbf{u}}{\partial t} = \begin{pmatrix} D_u & 0 \\ 0 & D_v \end{pmatrix} \Delta \mathbf{u} + \mathbf{f}(\mathbf{u})$$

where the Laplacian operator $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$. To first order in $\mathbf{u}_1$ and expanded about the steady state solution, the equation of motion is

$$\frac{\partial \mathbf{u}_1}{\partial t} = \begin{pmatrix} D_u & 0 \\ 0 & D_v \end{pmatrix} \Delta \mathbf{u}_1 + \mathbf{Df}\Big|_{\mathbf{u}_0} \mathbf{u}_1.$$

With trial solution $\mathbf{u}_1 = \tilde{\mathbf{u}}_1 e^{\gamma t + i\mathbf{k}\cdot\mathbf{x}}$ with $\mathbf{k} = (k_x, k_y)$ and $\mathbf{x} = (x, y)$ the first order equation gives

$$\gamma \tilde{\mathbf{u}}_1 = \left[- \begin{pmatrix} D_u & 0 \\ 0 & D_v \end{pmatrix} k^2 + \mathbf{Df}\Big|_{\mathbf{u}_0} \right] \tilde{\mathbf{u}}_1.$$

This can be rewritten with an identity matrix $\mathbf{I}$

$$\left[- \begin{pmatrix} D_u & 0 \\ 0 & D_v \end{pmatrix} k^2 + \mathbf{Df}\Big|_{\mathbf{u}_0} - \gamma \mathbf{I} \right] \tilde{\mathbf{u}}_1 = 0$$

The thing inside the brackets is a matrix. We find the characteristic equation by taking the determinant of the matrix and setting it to zero;

$$\det \left[\begin{pmatrix} \gamma + D_u k^2 & 0 \\ 0 & \gamma + D_v k^2 \end{pmatrix} - \mathbf{Df}\Big|_{\mathbf{u}_0} \right] = 0.$$

For the Brusselator model and using equation 16 for the Jacobian matrix

$$\det \left[\begin{pmatrix} \gamma + D_u k^2 & 0 \\ 0 & \gamma + D_v k^2 \end{pmatrix} - \begin{pmatrix} \beta - 1 & \alpha^2 \\ -\beta & -\alpha^2 \end{pmatrix} \right] = 0$$
$$\left(\gamma + D_u k^2 - \beta + 1\right)\left(\gamma + D_v k^2 + \alpha^2\right) - \alpha^2 \beta = 0.$$

We find the same characteristic equation as we derived in the last section but using different notation. As discussed in the last section, solutions to the characteristic equation tell you whether small perturbations can grown. if the real part of $\gamma(k)$ is positive then perturbations with wavelength $2\pi/k$ are likely to grow. The linear analysis does not tell you what types of patterns (like dots or ridges or spirals) are likely to form.

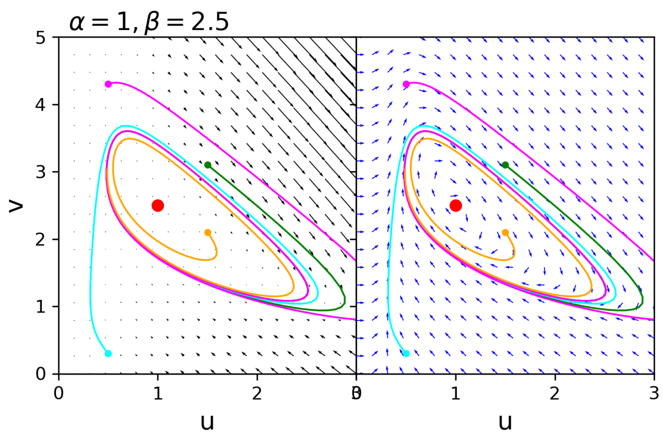

Figure 4: Trajectories in u, v space for the Brusselator model taking into account only evolution in u, v (without diffusion). The parameters $\alpha = 1, \beta = 2.5$. The fixed point is shown with a red dot and is unstable. Orbits are shown with colored lines. Arrows on the left show vectors $(\frac{du}{dt}, \frac{dv}{dt})$. Arrows on the right show the same vectors but normalized so that they all have the same length. Orbits are attracted to a limit cycle giving periodic behavior.

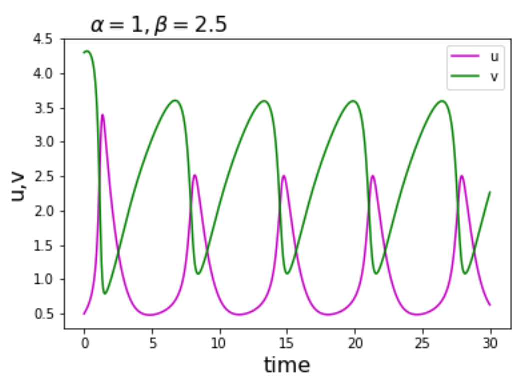

Figure 5: Time evolution of u, v in the Brusselator model for $\alpha = 1, \beta = 2.5$ showing a limit cycle.

1.3 Temporal behavior of the Brusselator model

We consider the Brusselator model at a single point and neglecting diffusion. The steady state solution may not be stable. Let us look at the Jacobian matrix computed at the steady state solution (equation 16) repeated here

$$\mathbf{J} = \mathbf{Df}\Big|_{\mathbf{u}_0} = \begin{pmatrix} \beta - 1 & \alpha^2 \\ -\beta & -\alpha^2 \end{pmatrix}. \tag{17}$$

We compute its trace and determinant

$$\begin{aligned} \text{tr}\mathbf{J} &= \beta - 1 - \alpha^2 \\ \det\mathbf{J} &= \alpha^2. \end{aligned} \tag{18}$$

We can compute the eigenvalues of this matrix. The eigenvalues of a 2x2 matrix in terms of its trace and determinant

$$\begin{aligned} \lambda_\pm &= \frac{1}{2}\left(\text{tr}A + \sqrt{\text{tr}A - 4\ \det A}\right) \\ &= \frac{1}{2}\left(\beta - 1 - \alpha^2 \pm \sqrt{(\beta - 1 - \alpha^2)^2 - 4\alpha^2}\right). \end{aligned} \tag{19}$$

The trace is the sum of the two eigenvalues and the determinant is the product of the two eigenvalues. If both trace and determinant are positive the fixed point is a repeller and is not stable.

Equations 18 and 19 show that the fixed point is unstable with positive real parts for both eigenvalues if $\text{tr}\mathbf{J} > 0$. This condition is

$$\beta - 1 - \alpha^2 > 0 \tag{20}$$

or equivalently

$$\beta > 1 + \alpha^2. \tag{21}$$

If the two eigenvalues are complex then the unstable fixed point has circulation and can give birth to a limit cycle (see Figures 4 and 5) . The eigenvalues have a complex part if the quantity inside the square root (in equation 19) is negative or

$$2\alpha > \beta - 1 - \alpha^2,$$

where I assumed the sign for $(\beta - 1 - \alpha^2)$ giving instability from equation 20. Equivalently for the eigenvalues to have complex parts we require

$$\beta < (1 + \alpha)^2. \tag{22}$$

Combining equations 21 and 22, the fixed point is both unstable and has complex eigenvalues, (giving birth to a limit cycle and with what is known as a *Hopf bifurcation*) if

$$1 + \alpha^2 > \beta > (1 + \alpha)^2. \tag{23}$$

We will get interesting temporal behavior in the Brusselator model if this condition is satisfied.

We should have discussed the global morphology of the system. For a limit cycle to appear, the dynamical system must be sufficiently non-linear that distant from the fixed point, trajectories move or contract toward the fixed point. We could make a quiver plot of the vector $\dot{u}, \dot{v}$ on the u, v plane to show that trajectories tend to circulate and move inwards at large values of u, v. Then orbits move away from the fixed point near the fixed point and move toward it at large distances from it. The attracting stable trajectory is a **limit cycle** which looks like a loop on the u, v plane, as shown in Figure 4 and gives periodic behavior for u and v, as shown in Figure 5.

1.4 Numerical implementation

We model the system discretely in both space and time.

In two dimensions we make an evenly spaced grid for the u, v values. The 2-dimensional spatial grid is specified by indices i, j where $i = 0, 1, ..., N-1$ and $j = 0, 1, ..., N-1$ for an $N \times N$ grid. The value of u at the i, j grid point is u_{ij} and the value of v is v_{ij}. The distance between consecutive grid points in either x or y directions is Δx.

We also discretize the system in time. We specify u, v values at evenly spaced times or separated in time by a time-step Δt. The value of u_{ij} at the n-th time-step is u_{ij}^n.

On a 1 dimensional spatial grid we can approximate the second derivative

$$\frac{\partial^2 u_j}{\partial x^2} \approx \frac{u_{j+1} + u_{j-1} - 2u_j}{(\Delta x)^2}$$

The two dimensional Laplacian

$$\frac{\partial^2 u_{ij}}{\partial x^2} + \frac{\partial^2 u_{ij}}{\partial y^2} \approx \frac{u_{i,j+1} + u_{i,j-1} + u_{i+1,j} + u_{i-1,j} - 4u_{ij}}{(\Delta x)^2}$$

We can use an Eulerian scheme to update the grid at the next time step using the u, v values at the current time step. We approximate the time derivative

$$\frac{\partial u_{ij}^n}{\partial t} \approx \frac{u_{ij}^{n+1} - u_{ij}^n}{\Delta t}$$

This gives

$$u_{ij}^{n+1} = u_{ij}^n + \Delta t \ \frac{\partial u_{ij}^n}{\partial t}.$$

The time derivative on the right is specified by the right hand side for our equations of motion. The full scheme is then

$$\begin{aligned}
u_{ij}^{n+1} &= u_{ij}^n + \Delta t \left(D_u \frac{u_{i,j+1}^n + u_{i,j-1}^n + u_{i+1,j}^n + u_{i-1,j}^n - 4u_{ij}^n}{(\Delta x)^2} + f_u(u_{ij}^n, v_{ij}^n) \right) \\
v_{ij}^{n+1} &= v_{ij}^n + \Delta t \left(D_v \frac{u_{i,j+1}^n + u_{i,j-1}^n + u_{i+1,j}^n + u_{i-1,j}^n - 4u_{ij}^n}{(\Delta x)^2} + f_v(u_{ij}^n, v_{ij}^n) \right)
\end{aligned}$$

where f_u, f_v are the reaction rate functions. Starting with some initial conditions for u, v 2-dimensional arrays, we can using this equation to compute new arrays for u, v consecutively for each time-step.

1.4.1 Initial conditions

Reaction-diffusion equations can be quite sensitive to initial conditions. For the Brusselator model, I find I tend to get nice patterns with u, v small but randomly chosen. For example, u, v values on the grid chosen from uniform distributions in $[0, 0.05)$.

1.4.2 Boundary conditions

Boundary conditions can affect the behavior of the model. The easiest type of boundary condition to implement numerically is the periodic boundary condition where we take i and j modulo N (the grid length) when computing the Laplacian.

1.4.3 Numerical Stability

The scheme will not be be stable unless we keep

$$\Delta t \lesssim \frac{(\Delta x)^2}{\max(D_u, D_v)}$$

This can be shown using von-Neumann analysis, but physically this condition can be understood by considering the time it takes information to travel between grid cells. Diffusion coefficients have units of Length^2/Time and information on the grid travels with scaling similar to that of a random walk. For a random walk, the variance of a number of walkers (a distance squared) is proportional to time. The time required for the bulk of them to travel a particular distance depends on the square of this distance. If the diffusion coefficient is larger or/and the grid spacing is smaller, then the time step must be reduced for the scheme to be numerically stable. If the scheme is unstable you will probably notice because you will get zigzags in u and v and numerical values will then increase rapidly to ∞.

The condition is similar to the CFL condition for a hydrodynamic system where Δt should be lower than the time it takes for sound waves to travel between grid points.

1.5 The Gray-Scott model

The Gray-Scott model has

$$f_u(u, v) = -uv^2 + \alpha(1 - u) \tag{24}$$

$$f_v(u, v) = uv^2 - (\alpha + \beta)v \tag{25}$$

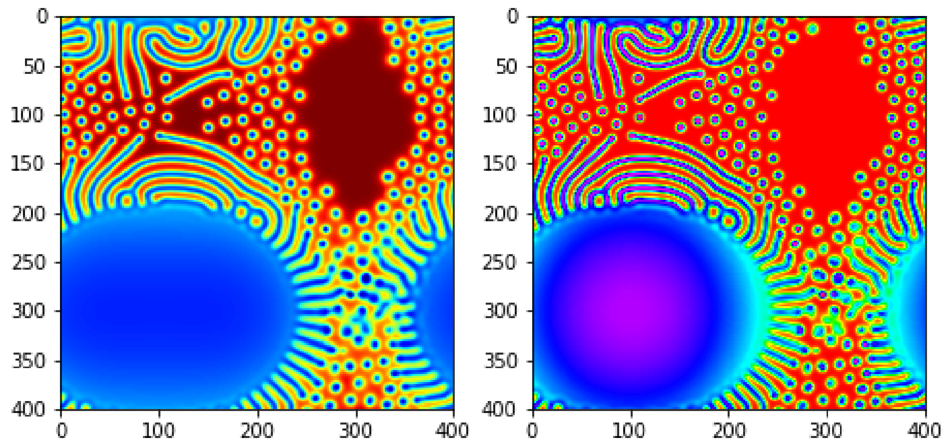

Figure 6: Patterns formed with the Gray-Scott model. u is on the left and v on the right. The grid has a sinusoidal variation in α (horizontally on the grid) and β (vertically on the grid). The mean values are $\alpha_m = 0.037$ and $\beta_m = 0.06$ with amplitudes of variation $\alpha_m/2$ and $\beta_m/8$. Diffusion coefficients are $D_u = 0.2, D_v = D_u/2$, the grid is $n = 400$ grid points and square and $\Delta x = \Delta t = 1$. Boundary conditions are periodic. The patterns grow but some regions of the plot (lower right) vary in time. In most regions, the patterns become fixed.

and

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + \alpha(1 - u) \tag{26}$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - (\alpha + \beta)v \tag{27}$$

α feeding rate for u and a drain rate for u, v. β gives a kill or drain rate for v. The uv^2 term is a reaction term, producing v at the expense of u. The Gray-Scott model, looks remarkably similar to the Brusselator model.

Nice initial conditions (giving patterns) for the Gray-Scott model are $u = 1$, $v = 0$ and some locations in the v array set to 1.

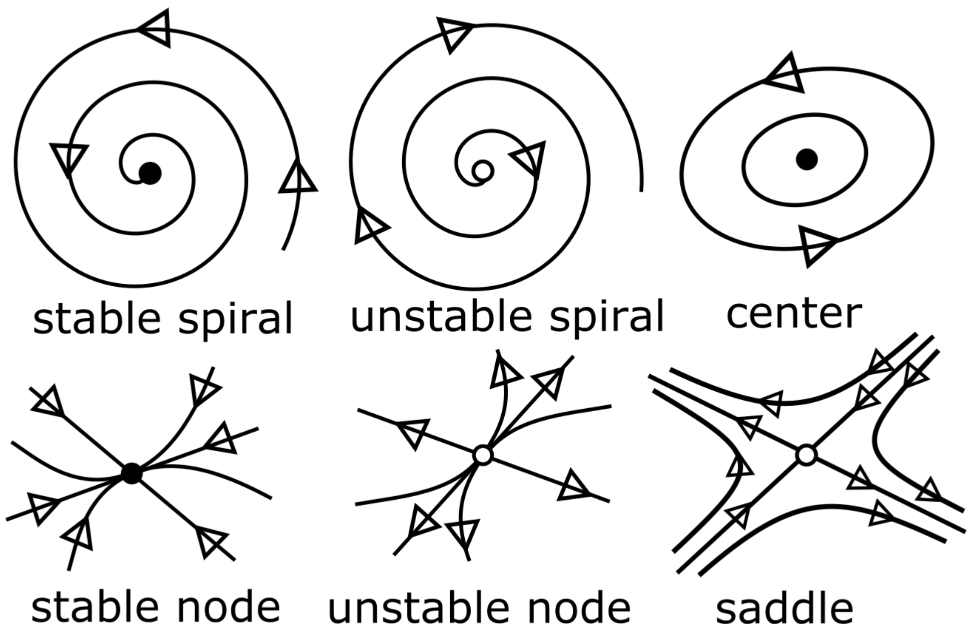

Figure 7: Different types of non-degenerate fixed points in 2-dimensional dynamical systems that are in the form $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$. The eigenvalues of the Jacobian matrix evaluated at the fixed point has imaginary components for the three systems in the top row. In the bottom row, both eigenvalues are different and real. Nodes are stable if the real part of both the eigenvalues are positive and unstable if they are both negative. If one eigenvalue is real and negative and the other is positive, the fixed point is a saddle node.

2 Stability of fixed points in a 2-dimensional dynamical system

A dynamical system on the (x, y) can be described with a trajectory $(x(t), y(t))$. Consider the system

$$\begin{aligned}\frac{dx}{dt} &= f(x, y)\\ \frac{dt}{dt} &= g(x, y)\end{aligned}$$

specified by two functions $f(x, y)$ and $g(x, y)$.

A fixed point (x_*, y_*) satisfies

$$\begin{aligned}f(x_*, y_*) &= 0\\ g(x_*, y_*) &= 0.\end{aligned} \tag{28}$$

We can look at the vicinity of the fixed point. Let's change variables to

$$\begin{aligned}x &= x_* + u\\ y &= y_* + v\end{aligned}$$

Because x_*, y_* are constants, $\frac{dx}{dt} = \frac{du}{dt}$ and $\frac{dy}{dt} = \frac{dv}{dt}$ The equation of motion becomes

$$\begin{aligned}\frac{du}{dt} &= f(x_* + u, y_* + v) \approx f(x_*, y_*) + u\frac{\partial f(x, y)}{\partial x}\bigg|_{(x_*,y_*)} + v\frac{\partial f(x, y)}{\partial y}\bigg|_{(x_*,y_*)}\\ \frac{dv}{dt} &= g(x_* + u, y_* + v) \approx g(x_*, y_*) + u\frac{\partial g(x, y)}{\partial x}\bigg|_{(x_*,y_*)} + v\frac{\partial g(x, y)}{\partial y}\bigg|_{(x_*,y_*)}\end{aligned}$$

Because (x_*, y_*) is a fixed point (equation 28) the equations of motion become

$$\begin{aligned}\frac{du}{dt} &= u\frac{\partial f(x, y)}{\partial x}\bigg|_{(x_*,y_*)} + v\frac{\partial f(x, y)}{\partial y}\bigg|_{(x_*,y_*)}\\ \frac{dv}{dt} &= u\frac{\partial g(x, y)}{\partial x}\bigg|_{(x_*,y_*)} + v\frac{\partial g(x, y)}{\partial y}\bigg|_{(x_*,y_*)}\end{aligned}$$

to first order in u, v. In vector notation

$$\mathbf{u} = \begin{pmatrix} u \\ v \end{pmatrix}.$$

The Jacobian matrix

$$\mathbf{J}(x,y) = \begin{pmatrix} \frac{\partial f(x,y)}{\partial x} & \frac{\partial f(x,y)}{\partial y} \\ \frac{\partial g(x,y)}{\partial x} & \frac{\partial g(x,y)}{\partial y} \end{pmatrix}.$$

In matrix form the equation of motion near the fixed point is the linear dynamical system

$$\frac{d\mathbf{u}}{dt} = \mathbf{J}_* \mathbf{u}$$

where the matrix $\mathbf{J}_* = \mathbf{J}(x_*, y_*)$ is evaluated at the fixed point.

This is a linear system and its behavior depends on the eigenvalues of the matrix $\mathbf{J}_*$. We assume a solution in the form $\mathbf{u} = e^{\lambda t}\mathbf{w}$ with $\mathbf{w}$ a constant vector. We insert this into the equation of motion to find

$$\lambda \mathbf{w} = \mathbf{J}_* \mathbf{w}. \tag{29}$$

This implies that λ is an eigenvalue of $\mathbf{J}_*$ and $\mathbf{w} = (u_w, v_w)$ is its accompanying eigenvector.

As the matrix is a 2x2 matrix, there are two eigenvalues λ_1, λ_2. If λ_1 is real and positive then trajectories exponentially diverge from the fixed point along the direction specified by its eigenvector. If both λ_1, λ_2 are real and positive then the fixed point is a *repeller* and is called an *unstable node*. If both λ_1, λ_2 are real and negative then the fixed point is an *attractor* and is called a *stable node*. If one of the eigenvalues is positive and the other is negative then the fixed point is a *saddle node* and nearby trajectories resemble hyperbolas.

Equation 29 can be rewritten using the identity matrix as

$$(\mathbf{J}_* - \lambda \mathbf{I})\,\mathbf{w} = \begin{pmatrix} \frac{\partial f}{\partial x} - \lambda & \frac{\partial f}{\partial y} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} - \lambda \end{pmatrix} \begin{pmatrix} u_w \\ v_w \end{pmatrix} = 0 \tag{30}$$

where the derivatives are evaluated at the fixed point. This has a solution if and only if the determinant of the matrix $\mathbf{J}_* - \lambda\mathbf{I}$ is zero;

$$\begin{vmatrix} \frac{\partial f}{\partial x} - \lambda & \frac{\partial f}{\partial y} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} - \lambda \end{vmatrix} = 0. \tag{31}$$

This gives the following equation which is called the *characteristic equation*

$$\lambda^2 - \left(\frac{\partial f}{\partial x} + \frac{\partial g}{\partial y}\right)\lambda + \frac{\partial f}{\partial x}\frac{\partial g}{\partial y} - \frac{\partial f}{\partial y}\frac{\partial g}{\partial x} = 0.$$

The characteristic equation can be written in terms of the trace of the Jacobian $\mathrm{tr}(\mathbf{J}_*)$ and the determinant of the Jacobian $\det(\mathbf{J}_*)$,

$$\lambda^2 - \mathrm{tr}(\mathbf{J}_*)\lambda + \det(\mathbf{J}_*) = 0.$$

The quadratic formula gives the eigenvalues

$$\lambda_1, \lambda_2 = \frac{1}{2}\mathrm{tr}(\mathbf{J}_*) \pm \frac{1}{2}\sqrt{(\mathrm{tr}(\mathbf{J}_*))^2 - 4\det \mathbf{J}_*}.$$

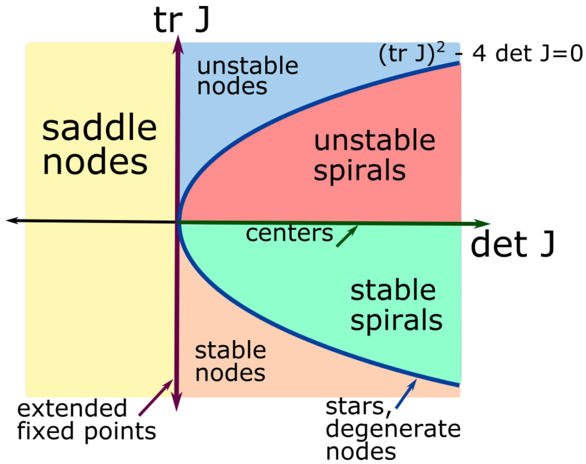

Figure 8: Classification of fixed points in 2-dimensional dynamical systems. J is the Jacobian matrix evaluated at the fixed point.

The general solution near the fixed point is

$$\mathbf{u} = \mathbf{c}_1 e^{\lambda_1 t}\mathbf{w}_1 + \mathbf{c}_2 e^{\lambda_2 t}\mathbf{w}_2$$

where $\mathbf{w}_1$ and $\mathbf{w}_2$ are the eigenvectors and constants $\mathbf{c}_1, \mathbf{c}_2$ are set by the initial condition. Note that there is a degenerate case; two eigenvectors might not exist.

If the eigenvalues have imaginary parts then these parts are equal and opposite in sign and there is rotation in the trajectories near the fixed point. If the real parts are positive and the eigenvectors have imaginary components then the fixed point is an unstable spiral or a spiral repeller. If the real parts are negative and the eigenvectors have imaginary components then the fixed point is a stable spiral node or a spiral attractor. If the eigenvalues are both imaginary (and the real parts are zero) then trajectories circle the fixed point and the motion resembles that of a harmonic oscillator. See Figure 7 for some illustrations of non-degenerate cases.

There are some other annoying details: If both eigenvalues are zero, then a whole region is full of fixed points. If one eigenvalue is zero, there is a line of fixed points. There are degenerate nodes that are at the boundary between spiral and not spiral. These can have only a single eigenvector direction. If both eigenvalues are the same and are non-zero and there are two eigenvectors then the trajectories look like a star. The entire range of possibilities is shown in Figure 8.

3 Hopf bifurcation and the birth of limit cycles

A Hopf Bifurcation is a kind of bifurcation that only occurs in a two dimensional dynamical system. A limit cycle is born from a fixed point that becomes unstable.

A Hopf bifurcation is a system that is sensitive to a parameter that we can vary. As the parameter is varied, the stability of the fixed point changes its nature and a periodic solution is born. The fixed point loses its stability.

The eigenvalues of the Jacobian must be complex when the fixed point is unstable. The fixed point becomes a spiral repeller. If the map distant from the fixed point contracts, a stable and attracting periodic orbit known as a **limit cycle** is born.

3.0.1 The van der Pol oscillator

An example of a dynamical system that exhibits a limit cycle is the van der Pol oscillator

$$\begin{aligned}\frac{dx}{dt} &= \mu(1-y^2)x - y \\ \frac{dx}{dt} &= x.\end{aligned} \tag{32}$$

The Jacobian matrix is

$$\mathbf{J}(x,y) = \begin{pmatrix} \mu(1-y^2) & -2\mu xy - 1 \\ 1 & 0 \end{pmatrix}. \tag{33}$$

The fixed point is at $(x,y) = (0,0)$. At the fixed point

$$\mathbf{J}(0,0) = \begin{pmatrix} \mu & -1 \\ 1 & 0 \end{pmatrix}. \tag{34}$$

Taking the determinant of $\mathbf{J}(0,0)$ we find the characteristic polynomial

$$\lambda^2 - \mu\lambda + 1 = 0,$$

which has solutions

$$\lambda_1, \lambda_2 = \frac{\mu}{2} \pm \frac{1}{2}\sqrt{\mu^2 - 4}. \tag{35}$$

See Figure 9 for the behavior of real and complex parts of the eigenvalues.

As long as $|\mu| < 2$ there is an imaginary part. If $0 < \mu < 2$ the real parts of the eigenvalues are positive, there are imaginary parts and the fixed point is an unstable spiral node. If $-2 < \mu < 0$ the real part of the eigenvalues are negative, there are imaginary parts and the fixed point is a stable spiral node.

The fixed point makes a transition from a stable to an unstable one at $\mu = 0$. We say the Hopf bifurcation occurs at $\mu = 0$. We can consider the trajectories of the two eigenvalues on the complex plane as μ is increased. The eigenvalues cross the imaginary axis when $\mu = 0$ (see Figure 9 right plot). The limit cycle only exists for $0 < \mu < 2$.

Take a look at Figures 4 and 5 showing limit cycles in the Brusselator model.

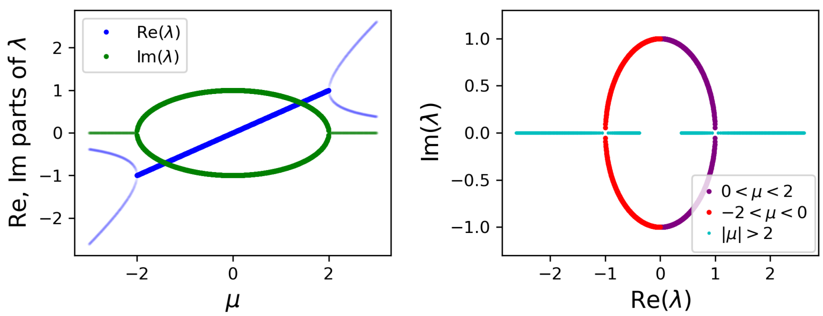

Figure 9: Eigenvalues of the Jacobian of the fixed point (computed using equation 35) of the van der Pol oscillator (with equation of motion in equation 32). Both eigenvalues are plotted on both plots. The Hopf bifurcation occurs at $\mu = 0$. For $0 < \mu < 2$ the fixed point is an unstable spiral, and the system exhibits a limit cycle.