Chapter 5

Reaction diffusion systems and pattern formation

5.1 Reaction diffusion systems from biology

In ecological problems, different species interact with each other, and in chemical reactions, different substances react and produce new substances. System of differential equations are used to model these events.

Similar to scalar reaction diffusion equations, reaction diffusion systems can be derived to model the spatial-temporal phenomena. Suppose that $U(t,x)$ and $V(t,x)$ are population density functions of two species or concentration of two chemicals, then the reaction diffusion system can be written as

$$\begin{aligned} \frac{\partial U}{\partial t} &= D_U \frac{\partial^2 U}{\partial x^2} + F(U,V), \\ \frac{\partial V}{\partial t} &= D_V \frac{\partial^2 V}{\partial x^2} + G(U,V), \end{aligned} \tag{5.1}$$

where D_U and D_V are the diffusion constants of U and V respectively, and $F(U,V)$ and $G(U,V)$ are the growth and interacting functions.

For simplicity, we only consider one-dimensional spatial domains. The domain can either be the whole space $(-\infty,\infty)$ when considering the spread or invasion of population in a new territory, or a bounded interval say $(0,L)$. In the latter case, appropriate boundary conditions need to be added to the system. Typically we consider the Dirichlet boundary condition (hostile exterior):

$$U(t,0) = U(t,L) = 0, \;\; V(t,0) = V(t,L) = 0, \tag{5.2}$$

or Neumann boundary condition (no-flux):

$$U_x(t,0) = U_x(t,L) = 0, \;\; V_x(t,0) = V_x(t,L) = 0. \tag{5.3}$$

The following are a list of models which has been studied by biologists and chemists:

Two species spatial ecological models:

Predator-prey:

$$U_t = D_U U_{xx} + A(U) - B(U,V), \;\; V_t = D_V V_{xx} - C(V) + kB(U,V). \tag{5.4}$$

Here U is a prey and V is a predator, $A(U)$ is the growth rate of U, $C(V)$ is the death rate of V, $k > 0$, and $B(U,V)$ is the interaction between U and V. Typical forms of these functions are

$$\begin{aligned} &A(U) = aU \text{ or } aU\left(1 - \frac{U}{N}\right), \;\; C(V) = cV, \\ &B(U,V) = dUV \text{ or } \frac{dUV}{1+eU}. \end{aligned} \tag{5.5}$$

Other ecological models are

Competition:

$$U_t = D_U U_{xx} + A(U) - B(U,V), \;\; V_t = D_V V_{xx} + C(V) - kB(U,V), \tag{5.6}$$

and

Mutualism:

$$U_t = D_U U_{xx} - A(U) + B(U,V), \;\; V_t = D_V V_{xx} - C(V) - kB(U,V). \tag{5.7}$$

Chemical reaction models: See more introduction in Murray's book.

Thomas mechanism

$$U_t = D_U U_{xx} + a - U - \rho R(U,V), \;\; V_t = D_V V_{xx} + c(b - V) - \rho R(U,V), \tag{5.8}$$

where $R(U,V) = \dfrac{dUV}{e + fU + gU^2}$. Thomas model is based on a specific reaction involving the substrates oxygen and uric acid which reacts in the presence of the enzyme uricase. U and V are the concentration of the uric acid and the oxygen respectively, and they are supplied at constant rates a and bc. Both U and V degrde linearly proportional to their concentrations, and both are used in the reaction at a rate of $\rho R(U,V)$. $R(U,V)$ is an empirical formula. For fixed V, $R(U,V)$ is nearly linear in U for small U, and it approached to zero as $U \to \infty$.

Schnakenberg reaction

$$U_t = D_U U_{xx} + a - bU + cU^2 V, \;\; V_t = D_V V_{xx} - d - cU^2 V. \tag{5.9}$$

This equation is from an artificial tri-molecular chemical reaction proposed by Schnakenberg:

$$X \rightleftharpoons^{k_1}_{k_{-1}} A, \;\; B \to^{k_2} Y, \;\; 2X + Y \to^{k_3} 3X, \tag{5.10}$$

Gierer-Meinhardt model

$$U_t = D_U U_{xx} + a - bU + c\frac{U^2}{V}, \quad V_t = D_V V_{xx} + dU^2 - eV. \tag{5.11}$$

Chlorine dioxide, iodine and malonic acid reaction (CIMA reaction)

$$U_t = D_U U_{xx} - s\left(a - U - \frac{4UV}{1+U^2}\right), \quad V_t = D_V V_{xx} + b\left(U - \frac{UV}{1+U^2}\right). \tag{5.12}$$

Gray-Scott model

$$U_t = D_U U_{xx} - U^2 V + f(1-U), \quad V_t = D_V V_{xx} + U^2 V - (f+k)V. \tag{5.13}$$

All these models can be rewritten to a standard form:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2} + \lambda f(u,v), \\ \frac{\partial v}{\partial t} &= d\frac{\partial^2 v}{\partial x^2} + \lambda g(u,v), \end{aligned} \tag{5.14}$$

after a nondimensionalization procedure.

5.2 Turing instability and pattern formation

We consider the nondimensionalized system

$$\begin{cases} u_t = u_{xx} + \lambda f(u,v), \quad t > 0, \ x \in (0,1), \\ v_t = d v_{xx} + \lambda g(u,v), \quad t > 0, \ x \in (0,1), \\ u_x(t,0) = u_x(t,1) = v_x(t,0) = v_x(t,1) = 0, \\ u(0,x) = a(x), \quad v(0,x) = b(x). \end{cases} \tag{5.15}$$

We suppose that (u_0, v_0) is a constant equilibrium solution, *i.e.*

$$f(u_0, v_0) = 0, \quad \text{and } g(u_0, v_0) = 0. \tag{5.16}$$

In fact, the constant solution (u_0, v_0) is also an equilibrium solution of a system of ordinary differential equations:

$$\begin{cases} u' = \lambda f(u,v), \quad t > 0, \\ v' = \lambda g(u,v), \quad t > 0, \\ u(0) = a, \quad v(0) = b. \end{cases} \tag{5.17}$$

In 1952, Alan Turing published a paper "The chemical basis of morphogenesis" which is now regarded as the foundation of basic chemical theory or reaction diffusion theory of morphogenesis. Turing suggested that, under certain conditions, chemicals can react and diffuse in such a way as to produce non-constant equilibrium solutions, which represent spatial patterns of chemical or morphogen concentration. It is noticeable that Alan Turing was one of the greatest scientists in twentieth century. He was responsible for much of the fundamental work that underlies the formal theory of computation, general purpose computer, and artificial intelligence. During World War II, Turing was a key figure in the successful effort to break the Axis Enigma code used in all German U-boats, which is one of the most important contributions scientists made to the victory of the war.

Turing's idea is a simple but profound one. He said that if, in the absence of the diffusion (considering ODE (5.17)), u and v tend to a linearly stable uniform steady state, then, under certain conditions, the uniform steady state can become unstable, and spatial inhomogeneous patterns can evolve through bifurcations. In another word, an constant equilibrium can be asymptotically stable with respect to (5.17), but it is unstable with respect to (5.15). Therefore this constant equilibrium solution becomes unstable because of the diffusion, which is called *diffusion driven instability*. Diffusion is usually considered a smoothing and stablising process, that is why this was such a novel concept. More information of Turing instability can be found in Murray's book Chapter 14.

So now we look for the conditions for the Turing instability described above. If (u_0, v_0) is stable with respect to (5.15), then the eigenvalues of Jacobian

$$J = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} \tag{5.18}$$

at (u_0, v_0) must all have negative real part, which is equivalent to

$$Trace(J) = f_u + g_v < 0, \quad Determinant(J) = f_u g_v - f_v g_u > 0. \tag{5.19}$$

Now suppose that (u_0, v_0) is unstable with respect to (5.17). Then (u_0, v_0) must also be unstable with respect to the linearized equation:

$$\begin{cases} \phi_t = \phi_{xx} + \lambda f_u(u_0, v_0)\phi + \lambda f_v(u_0, v_0)\psi, \quad t > 0, \ x \in (0, 1), \\ \psi_t = d\psi_{xx} + \lambda g_u(u_0, v_0)\phi + \lambda g_v(u_0, v_0)\psi, \quad t > 0, \ x \in (0, 1), \\ \phi_x(t, 0) = \phi_x(t, 1) = \psi_x(t, 0) = \psi_x(t, 1) = 0, \\ \phi(0, x) = c(x), \quad \psi(0, x) = d(x), \end{cases} \tag{5.20}$$

or in matrix notation:

$$\mathbf{\Psi}_t = D\mathbf{\Psi}_{xx} + \lambda J \mathbf{\Psi}, \tag{5.21}$$

where

$$\mathbf{\Psi}(t, x) = \begin{pmatrix} \phi(t, x) \\ \psi(t, x) \end{pmatrix}, \quad \text{and } D = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix}. \tag{5.22}$$

From the separation of variables for single equation, we expect that ϕ and ψ are both separable, and we try the following form:

$$\mathbf{\Psi}(t, x) = \begin{pmatrix} \phi(t, x) \\ \psi(t, x) \end{pmatrix} = \begin{pmatrix} u_k(t) \\ v_k(t) \end{pmatrix} \cos(k\pi x) = \mathbf{W}_k(t)\cos(k\pi x). \tag{5.23}$$

We shall try this form of solution, and the general solution for $\mathbf{\Psi}$ would be

$$\mathbf{\Psi}(t,x) = \sum_{k=0}^{\infty} \mathbf{W}_k(t)\cos(k\pi x) \tag{5.24}$$

By substitution of this form into (5.21), we obtain that $\mathbf{W}_k(t)$ satisfies a system of ordinary differential equations:

$$\frac{d\mathbf{W}_k}{dt} = (\lambda J - k^2\pi^2 D)\mathbf{W}_k. \tag{5.25}$$

If (5.20) is an unstable system, then at least one of $\mathbf{W}_k(t)$ would go to infinity as $t \to \infty$, *i.e.* one of the eigenvalues of matrix $M_k = \lambda J - k^2\pi^2 D$ has positive real part. The eigenvalues μ_1 and μ_2 of $\lambda J - k^2\pi^2 D$ satisfy

$$\begin{aligned} &\mu^2 - [\lambda(f_u + g_v) - (d+1)k^2\pi^2]\mu \\ &+(f_u g_v - f_v g_u)\lambda^2 - k^2\pi^2(df_u + g_v)\lambda + dk^4\pi^4 = 0, \end{aligned} \tag{5.26}$$

and

$$\begin{aligned} &Trace(M_k) = \lambda(f_u + g_v) - (d+1)k^2\pi^2, \\ &Determinant(M_k) = (f_u g_v - f_v g_u)\lambda^2 - k^2\pi^2(df_u + g_v)\lambda + dk^4\pi^4. \end{aligned} \tag{5.27}$$

Since $f_u + g_v < 0$, then $Trace(M_k) < 0$ is always true. So M_k cannot be a source or spiral source. If M_k is unstable, then it can only be a saddle. Therefore we must have $Determinant(M_k) < 0$.

Remember that we only need one of M_k is unstable. So let's take a look of the values of $h(k^2\pi^2) = Determinant(M_k)$ for different k (or $k^2\pi^2$ indeed.) Here we define the function

$$h(w) = (f_u g_v - f_v g_u)\lambda^2 - w(df_u + g_v)\lambda + dw^2. \tag{5.28}$$

When $w = 0$, $h(0) = (f_u g_v - f_v g_u)\lambda^2 > 0$ because we require $f_u g_v - f_v g_u > 0$, and when $k^2\pi^2$ is large ($\to \infty$), we also have $\lim_{w\to\infty} h(w) = \infty$. So we must hope that for some $0 < k^2\pi^2 < \infty$, $h(k^2\pi^2) < 0$. Since h is a quadratic equation, we must require $\min_{w\geq 0} h(w) < 0$. It is easy to calculate that $\min_{w\geq 0} h(w)$ is achieved at $w_0 = \dfrac{df_u + g_v}{2d}$. This implicitly implies that

$$df_u + g_v > 0, \tag{5.29}$$

otherwise $h(w) > 0$ for all $w \geq 0$. The minimum value at w_0 is

$$h(w_0) = \lambda^2\left(f_u g_v - f_v g_u - \frac{(df_u + g_v)^2}{4d}\right), \tag{5.30}$$

which must be negative, so

$$(df_u + g_v)^2 - 4d(f_u g_v - f_v g_u) > 0. \tag{5.31}$$

Summarizing all conditions we got so far, if (u_0, v_0) is stable with respect to (5.15) but unstable with respect to (5.17), then d and J must satisfy

$$\begin{aligned} &f_u + g_v < 0, \quad f_u g_v - f_v g_u > 0, \\ &df_u + g_v > 0, \quad (df_u + g_v)^2 - 4d(f_u g_v - f_v g_u) > 0. \end{aligned} \tag{5.32}$$

The conditions in (5.32) give the range of parameter d such that (u_0, v_0) is possibly unstable, but only (5.32) can only assure that certain values of $h(w)$ are negative, but it cannot guarantee there is a value $k^2\pi^2$ such that $h(k^2\pi^2) < 0$. To achieve that, we directly calculate the conditions for $h(k^2\pi^2) < 0$. From (5.28), we have

$$h(k^2\pi^2) = (f_u g_v - f_v g_u)\lambda^2 - k^2\pi^2(df_u + g_v)\lambda + dk^4\pi^4 < 0, \tag{5.33}$$

and if $f_u > 0$ and $g_v < 0$, then

$$d > \frac{\lambda(D\lambda - k^2\pi^2 g_v)}{k^2\pi^2(f_u\lambda - k^2\pi^2)} \equiv d_k(\lambda), \tag{5.34}$$

where $D = f_u g_v - f_v g_u$. $\{d_k(\lambda)\}$ is a family of curves with $d_k(\lambda)$ defined on $(k^2\pi^2/f_u, \infty)$ (see example below.) For a pair of parameters (λ, d), if $d > d_k(\lambda)$ for some natural number k, then (u_0, v_0) is unstable. But if $d < d_k(\lambda)$ for any k, then it is stable. Summarizing the above calculation, we conclude

Theorem 5.1. *Suppose that (u_0, v_0) is a constant equilibrium solution of the reaction diffusion system*

$$\begin{cases} u_t = u_{xx} + \lambda f(u,v), & t > 0,\ x \in (0,1), \\ v_t = dv_{xx} + \lambda g(u,v), & t > 0,\ x \in (0,1), \\ u_x(t,0) = u_x(t,1) = v_x(t,0) = v_x(t,1) = 0, \\ u(0,x) = a(x), \quad v(0,x) = b(x), \end{cases} \tag{5.35}$$

and the Jacobian of (f,g) at (u_0,v_0) is $J(u_0,v_0) = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}$. If J, d and λ satisfy

$$\begin{aligned} &f_u > 0,\ g_v < 0,\ f_u + g_v < 0,\ \ f_u g_v - f_v g_u > 0, \\ &df_u + g_v > 0,\ \ (df_u + g_v)^2 - 4d(f_u g_v - f_v g_u) > 0, \end{aligned} \tag{5.36}$$

and $d > d_k(\lambda)$ for some k, where

$$d_k(\lambda) = \frac{\lambda(D\lambda - k^2\pi^2 g_v)}{k^2\pi^2(f_u\lambda - k^2\pi^2)}, \quad D = f_u g_v - f_v g_u, \tag{5.37}$$

then (u_0, v_0) is an unstable equilibrium solution with respect to (5.35), but a stable equilibrium solution with respect to $u' = \lambda f(u,v)$, $v' = \lambda g(u,v)$.

We use the example of Schnackenberg to illustrate the theorem. Consider the following and a nondimensionalized system of reaction diffusion equations describing the chemical reaction is

$$\begin{cases} u_t = u_{xx} + \lambda(a - u + u^2 v), & t > 0,\ x \in (0,1), \\ v_t = dv_{xx} + \lambda(b - u^2 v), & t > 0,\ x \in (0,1), \\ u_x(t,0) = u_x(t,1) = v_x(t,0) = v_x(t,1) = 0, \\ u(0,x) = A_0(x), \quad v(0,x) = B_0(x), \end{cases} \tag{5.38}$$

where $a, b > 0$. There is a unique equilibrium constant solution (u_0, v_0) such that

$$u_0 = a + b, \quad v_0 = \frac{b}{(a+b)^2}, \tag{5.39}$$

and the Jacobian at (u_0, v_0) is

$$J(u_0, v_0) = \begin{pmatrix} \dfrac{b-a}{b+a} & (b+a)^2 \\ -\dfrac{2b}{b+a} & -(b+a)^2 \end{pmatrix} \tag{5.40}$$

Then from simple computation, the conditions (5.36) become

$$\begin{aligned} &0 < b - a < (b+a)^3, \quad (b+a)^2 > 0, \\ &d(b-a) > (b+a)^3, \quad [d(b-a) - (b+a)^3]^2 > 4d(b+a)^4. \end{aligned} \tag{5.41}$$

For simplicity and transparency of the result, we select a pair of $(a, b) = (1, 2)$, then the first row of (5.41) is satisfied. The formula for $d_k(\lambda)$ in this case is

$$d_k(\lambda) = \frac{27\lambda(\lambda + k^2\pi^2)}{k^2\pi^2(\lambda - 3k^2\pi^2)}. \tag{5.42}$$

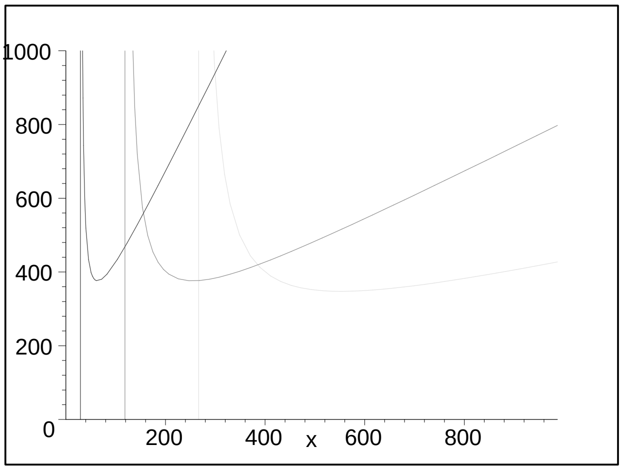

Figure 5.1: Parameter space (λ, d) for Turing instability

The first three $d_k(\lambda)$ are drawn in Fig. 5.1. Each $d_k(\lambda)$ is a concave up curve with a unique minimum point. From Theorem 5.1, if (λ, d) falls below all of $d_k(\lambda)$, then (u_0, v_0) is stable for that parameter choice; and if (λ, d) is above any of $d_k(\lambda)$, then (u_0, v_0) is unstable.

When (u_0, v_0) is unstable, the solution of linearized equation (5.20) has a form

$$\mathbf{\Psi}(t, x) = \sum_{k=0}^{\infty} (c_{1k} e^{\mu_{1k} t} \mathbf{W}_{1k} + c_{2k} e^{\mu_{2k} t} \mathbf{W}_{2k}) \cos(k\pi x), \tag{5.43}$$

where μ_{1k} and μ_{2k} are the eigenvalues of $\lambda J - k^2\pi^2 D$, and $\mathbf{W}_{1k}$, $\mathbf{W}_{2k}$ are corresponding eigenvectors. Since it is unstable, then one or more eigenvalues μ_{1k} or μ_{2k} are positive. For example, if (λ, d) is a point such that $d > d_2(\lambda)$ but $d < d_k(\lambda)$ for all other k, then there is one eigenvalue $\mu_{12} > 0$ (or complex with positive real part), and all other eigenvalues have negative real part, and as $t \to \infty$,

$$\mathbf{\Psi}(t,x) \approx c_{12} e^{\mu_{12} t} \mathbf{W}_{12}(t) \cos(2\pi x). \tag{5.44}$$

So the solution grows exponentially as $t \to \infty$, and it grows in a temporal-spatial pattern $\mathbf{W}_{1k}(t)\cos(2\pi x)$, which is called an *unstable mode* of this equilibrium solution. For an unstable equilibrium, there may be more than one unstable modes if the parameter pair (λ, d) is below two curves $d_k(\lambda)$.

The linear analysis of Turing instability is completed now. For nonlinear systems, if the initial value is near the constant equilibrium solution, then in a short time, the orbit would be close to that of linearized equation. When the equilibrium is unstable, a spatial pattern is formed following its unstable mode, and the pattern grows exponentially fast for a short period. But after that, the nonlinear structure takes over, and usually nonlinear functions force the solutions staying bounded (like in the logistic model), thus the solution approaches a bounded spatial pattern as $t \to \infty$. Although the mechanism of the nonlinear evolution is still not clear mathematically, people believe that the spatial pattern formed in the earlier stage near equilibrium solution is kept, which seems to be supported by numerical simulations. Many problems are still topics of current research interests. More biological discussion can be found in Murray's book page 388-414.

5.3 Turing patterns in 2-D and animal coat patterns

5.4 Chemotactic motion of microorganisms

5.5 Spatial epidemic model

Chapter 5 Exercises

1. Consider the diffusive predator-prey model

$$\begin{cases} \dfrac{\partial U}{\partial t} = D_U \dfrac{\partial^2 U}{\partial x^2} + AU - BUV, \quad s > 0,\ y \in (0, L), \\ \dfrac{\partial V}{\partial t} = D_V \dfrac{\partial^2 V}{\partial x^2} - CV + DUV, \quad s > 0, y \in (0, L), \\ \dfrac{\partial U}{\partial y}(t,0) = \dfrac{\partial U}{\partial y}(t,L) = \dfrac{\partial V}{\partial y}(t,0) = \dfrac{\partial V}{\partial y}(t,L) = 0, \\ U(0,y) = U_0(y), \quad V(0,y) = V_0(y). \end{cases} \tag{5.45}$$

Use the substitution

$$t = \frac{D_U}{L^2} s,\ x = \frac{y}{L},\ u = \frac{B}{A} U,\ v = \frac{D}{C} V,$$

to show the nondimensionalized equation has the form

$$\begin{cases} u_t = u_{xx} + \lambda[Au - (C/D)uv], \;\; t > 0, \; x \in (0,1), \\ v_t = dv_{xx} + \lambda[-Cv + (A/B)uv], \;\; t > 0, \; x \in (0,1), \\ u_x(t,0) = u_x(t,1) = v_x(t,0) = v_x(t,1) = 0, \\ u(0,x) = u_0(x), \;\; v(0,x) = v_0(x). \end{cases} \tag{5.46}$$

Express the new parameters d and λ in terms of old parameters.

2. Consider Gierer-Meinhardt system:

$$\begin{cases} u_t = u_{xx} + \lambda(-0.5u + \dfrac{u^2}{v}), \;\; t > 0, \; x \in (0,1), \\ v_t = dv_{xx} + \lambda(-v + u^2), \;\; t > 0, \; x \in (0,1), \\ u_x(t,0) = u_x(t,1) = v_x(t,0) = v_x(t,1) = 0, \\ u(0,x) = A_0(x), \;\; v(0,x) = B_0(x). \end{cases} \tag{5.47}$$

Apply Theorem 5.1, and determine the regions in (λ, d) plane where the equilibrium $(u_0, v_0) = (1, 1)$ is linearly unstable.

3. In (5.38) with $(a, b) = (1, 2)$, we assume that $\lambda = 4\pi^2$ and $0 < d < \infty$. From Fig. 5.1, there is a unique $d_1 = d_1(4\pi^2)$ such that (u_0, v_0) is stable when $d < d_1$ and it is unstable with unstable mode $\cos(\pi x)$ when $d > d_1$. At $d = d_1$, a bifurcation occurs. Use perturbation method to calculate the bifurcating solutions when d is near d_1, and determine the types of bifurcation (subcritical, supercritical, transcritical, pitchfork, etc.)