

Autocatalytic Reaction-Diffusion Models and Travelling Waves

Mathematical Modelling Week 7

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Modelling Autocatalytic Reactions

Consider a chemical species A dissolved in some solvent in a one-dimensional vessel, say from $x = 0$ to $x = 1$. Let $u(x, t)$ be the concentration of A . It's reasonable to assume that A diffuses with some diffusivity κ . If the amount of A were conserved we would have $u_t - \kappa u_{xx} = 0$. If the chemical A can't leave the vessel at the endpoints then we'd also have $u_x(0, t) = u_x(1, t) = 0$.

But suppose that A IS being created in the vessel, say from other chemical species. Let's suppose also that the rate at which A is created (on a per time per length basis) depends ONLY on the current concentration of A itself and not explicitly any other factors. In this case rate of production of A is given by some function $F(u)$. Such reactions are called *autocatalytic*, if the presence of the chemical A stimulates the production of more of A .

Exercises

1. Write out the PDE (involving F) satisfied by $u(x, t)$ for such an autocatalytic reaction.
2. What should we choose for F ? That depends on the specifics of the reaction, but here's a start: We should require F to satisfy $F(0) = 0$ (no A present, none produced). Also, suppose that A can only be produced up to some maximum concentration, say m , after which the production rate falls to zero (and maybe then goes negative).

Find a simple function $F(u)$ (defined for $u \geq 0$) that satisfies these criteria. Hint: an autocatalytic reactant is like a reproducing animal.

Chemical and Biological Waves

Equations of the form $u_t - \kappa u_{xx} = F(u)$ don't typically have closed form solutions, so we have to resort to numerics. However, there is an important class of solutions to these type of problems that have physical significance.

They are the so-called *travelling wave* solutions, and they model the propagation of chemical reaction “waves”, in the context of autocatalytic reactions, or “infestation waves” if the DE models the propagation of some (pest) species. Such DE’s also come up in genetics to model the spread of genes throughout a population.

We’re going to consider the equation $u_t - u_{xx} = F(u)$ on the entire real line $-\infty < x < \infty$, and we’ll look at the specific case $F(u) = u(1 - u)$. Note also I set the diffusivity equal to one. A travelling wave solution to $u_t - u_{xx} = u(1 - u)$ means a solution of the form

$$u(x, t) = \phi(x - ct) \tag{1}$$

for some constant c , the wave speed. This looks just like a solution to the advection equation, which is quite different from diffusion. We’ll look for right moving waves, so $c > 0$ (left moving is the same idea). We will require also that ϕ remain bounded. If we plug $u(x, t) = \phi(x - ct)$ into $u_t - u_{xx} = u(1 - u)$ we find that ϕ must satisfy an ODE

$$-c\phi'(s) - \phi''(s) = (1 - \phi(s))\phi(s) \tag{2}$$

(where $s = x - ct$). We need to find a solution to this ODE which remains bounded for $-\infty < s < \infty$.

Let $x_1 = \phi$ and $x_2 = \phi'$. Then equation (2) is equivalent to the nonlinear ODE system

$$x_1' = x_2 \tag{3}$$

$$x_2' = -(1 - x_1)x_1 - cx_2. \tag{4}$$

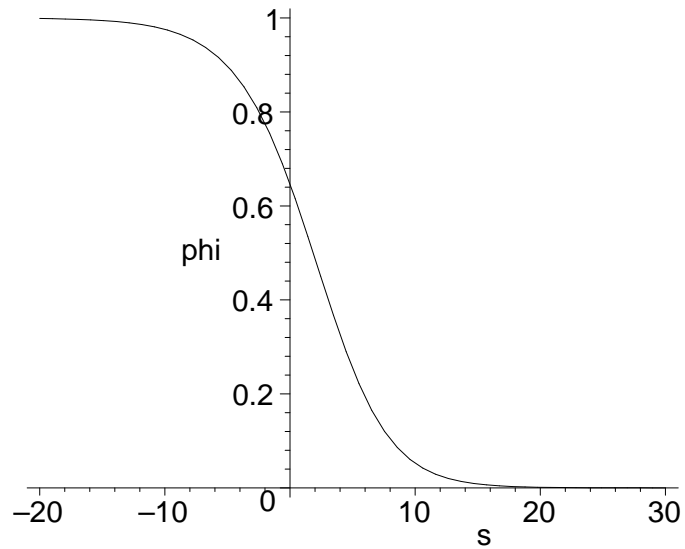
Time to recall some DE 2! You can sketch a phase portrait for this system. First, the fixed points are the point $(0, 0)$ and $(1, 0)$ in the x_1x_2 plane. The eigenvalues for the linearized system at $(0, 0)$ are $\frac{1}{2}(-c \pm \sqrt{c^2 - 4})$. Now if $c^2 < 4$ these are complex with negative real part, so $(0, 0)$ is a stable spiral. If $c^2 \geq 4$ then $(0, 0)$ is still stable, (a stable node). The eigenvalues for the fixed point at $(1, 0)$ are $\frac{1}{2}(-c \pm \sqrt{c^2 + 4})$. One eigenvalue is always positive, the other negative, so $(1, 0)$ is ALWAYS a saddle point. A typical phase portrait for $c > 2$ looks like

We need to pick out a solution $(x_1(s), x_2(s))$, that remains bounded for all s . If you look at the phase portrait, you'll see there's only one candidate (which I sketched), namely the solution that approaches $(1, 0)$ as $s \rightarrow -\infty$ and $(0, 0)$ as $s \rightarrow \infty$. Now if $0 < c < 2$ this solution will spiral around $(0, 0)$, but if $c \geq 2$ the solution will “dive” straight in. There a slight problem with taking $c < 2$ —see the exercise below.

The solution $\phi(s)$ satisfies $\lim_{s \rightarrow -\infty} \phi(s) = 1$ and $\lim_{s \rightarrow \infty} \phi(s) = 0$. Note also that $\phi' = x_2$ limits to zero in both directions. The function

$$u(x, t) = \phi(x - ct)$$

is a travelling wave solution to $u_t - u_{xx} = u(1 - u)$. Most amazingly, note we can construct travelling wave solutions with ANY wave speed $c \geq 2$. Here's a picture of $\phi(s)$ for $c = 3$.



As it turns out, these travelling wave solutions are stable, in the sense that if you start the PDE with initial data close enough to such a travelling wave, it will approach the travelling wave solution.

Exercises:

1. If we take $0 < c < 2$ the solutions to equations (3) will spiral around the origin. In the context in which u represents a population density or chemical density, what's wrong with this?
2. Show that this analysis holds true for any reaction-diffusion equation $u_t - u_{xx} = F(u)$ as long as F has the properties $F(0) = 0$, $F(m) = 0$, $F(u) > 0$ for $0 < u < m$, and $F(u) < 0$ for either $u < 0$ or $u > m$.