LECTURE 1

Introduction

> The source of all great mathematics is the special case, the concrete example. It is frequent in mathematics that every instance of a concept of seemingly great generality is in essence the same as a small and concrete special case.[1]

We begin by describing a rather general framework for the derivation of PDEs that describe the conservation, or balance, of some quantity.

1. Conservation laws

We consider a quantity $\mathcal{Q}$ that varies in space, $\vec{x}$, and time, t, with density $u(\vec{x}, t)$, flux $\vec{q}\,(\vec{x}, t)$, and source density $\sigma\,(\vec{x}, t)$.

For example, if $\mathcal{Q}$ is the mass of a chemical species diffusing through a stationary medium, we may take u to be the density, $\vec{q}$ the mass flux, and f the mass rate per unit volume at which the species is generated.

For simplicity, we suppose that $u(x, t)$ is scalar-valued, but exactly the same considerations would apply to a vector-valued density (leading to a system of equations).

1.1. Integral form

The conservation of $\mathcal{Q}$ is expressed by the condition that, for any fixed spatial region Ω, we have

$$\frac{d}{dt}\int_{\Omega} u\, d\vec{x} = -\int_{\partial\Omega} \vec{q}\cdot\vec{n}\, dS + \int_{\Omega} \sigma\, d\vec{x}. \tag{1.1}$$

Here, $\partial\Omega$ is the boundary of Ω, $\vec{n}$ is the unit outward normal, and dS denotes integration with respect to surface area.

Equation (1.1) is the integral form of conservation of $\mathcal{Q}$. It states that, for any region Ω, the rate of change of the total amount of $\mathcal{Q}$ in Ω is equal to the rate at which $\mathcal{Q}$ flows into Ω through the boundary $\partial\Omega$ plus the rate at which $\mathcal{Q}$ is generated by sources inside Ω.

1.2. Differential form

Bringing the time derivative in (1.1) inside the integral over the fixed region Ω, and using the divergence theorem, we may write (1.1) as

$$\int_{\Omega} u_t\, d\vec{x} = \int_{\Omega} \left(-\nabla\cdot\vec{q} + \sigma\right)\, d\vec{x}$$

[1] P. Halmos.

Since this equation holds for arbitrary regions Ω, it follows that, for smooth functions,

$$u_t = -\nabla \cdot \vec{q} + \sigma. \tag{1.2}$$

Equation (1.2) is the differential form of conservation of $\mathcal{Q}$.

When the source term σ is nonzero, (1.2) is often called, with more accuracy, a balance law for $\mathcal{Q}$, rather than a conservation law, but we won't insist on this distinction.

2. Constitutive equations

The conservation law (1.2) is not a closed equation for the density u. Typically, we supplement it with constitutive equations that relate the flux $\vec{q}$ and the source density σ to u and its derivatives. While the conservation law expresses a general physical principle, constitutive equations describe the response of a particular system being modeled.

Example 1.1. If the flux and source are pointwise functions of the density,

$$\vec{q} = \vec{f}(u), \qquad \sigma = g(u),$$

then we get a first-order system of PDEs

$$u_t + \nabla \cdot \vec{f}(u) = g(u).$$

For example, in one space dimension, if $g(u) = 0$ and $f(u) = u^2/2$, we get the inviscid Burgers equation

$$u_t + \left(\frac{1}{2}u^2\right)_x = 0.$$

This equation is a basic model equation for hyperbolic systems of conservation laws, such as the compressible Euler equations for the flow of an inviscid compressible fluid [**47**].

Example 1.2. Suppose that the flux is a linear function of the density gradient,

$$\vec{q} = -A\nabla u, \tag{1.3}$$

where A is a second-order tensor, that is a linear map between vectors. It is represented by an $n \times n$ matrix with respect to a choice of n basis vectors. Then, if $\sigma = 0$, we get a second order, linear PDE for $u(\vec{x}, t)$

$$u_t = \nabla \cdot (A\nabla u)\,. \tag{1.4}$$

Examples of this constitutive equation include: Fourier's law in heat conduction (heat flux is a linear function of temperature gradient); Fick's law (flux of solute is a linear function of the concentration gradient); and Darcy's law (fluid velocity in a porous medium is a linear function of the pressure gradient). It is interesting to note how old each of these laws is: Fourier (1822); Fick (1855); Darcy (1855).

The conductivity tensor A in (1.3) is usually symmetric and positive-definite, in which case (1.4) is a parabolic PDE; the corresponding PDE for equilibrium density distributions $u(\vec{x})$ is then an elliptic equation

$$\nabla \cdot (A\nabla u) = 0.$$

In general, the conductivity tensor may depend upon $\vec{x}$ in a nonuniform system, and on u in non-linearly diffusive systems. While A is almost always symmetric, it need not be diagonal in an anisotropic system. For example, the heat flux in a crystal lattice or in a composite medium made up of alternating thin layers of copper and asbestos is not necessarily in the same direction as the temperature gradient.

For a uniform, isotropic, linear system, we have $A = \nu I$ where ν is a positive constant, and then $u(\vec{x}, t)$ satisfies the heat, or diffusion, equation

$$u_t = \nu \Delta u.$$

Equilibrium solutions satisfy Laplace's equation

$$\Delta u = 0.$$

3. The KPP equation

In this section, we discuss a specific example of an equation that arises as a model in population dynamics and genetics.

3.1. Reaction-diffusion equations

If $\vec{q} = -\nu \nabla u$ and $\sigma = f(u)$ in (1.2), we get a *reaction-diffusion* equation

$$u_t = \nu \Delta u + f(u).$$

Spatially uniform solutions satisfy the ODE

$$u_t = f(u),$$

which is the 'reaction' equation. In addition, diffusion couples together the solution at different points.

Such equations arise, for example, as models of spatially nonuniform chemical reactions, and of population dynamics in spatially distributed species.

The combined effects of spatial diffusion and nonlinear reaction can lead to the formation of many different types of spatial patterns; the spiral waves that occur in Belousov-Zabotinski reactions are one example.

One of the simplest reaction-diffusion equations is the KPP equation (or Fisher equation)

$$u_t = \nu u_{xx} + ku(a - u). \tag{1.5}$$

Here, ν, k, a are positive constants; as we will show, they may be set equal to 1 without loss of generality.

Equation (1.5) was introduced independently by Fisher [**22**], and Kolmogorov, Petrovsky, and Piskunov [**33**] in 1937. It provides a simple model for the dispersion of a spatially distributed species with population density $u(x, t)$ or, in Fisher's work, for the advance of a favorable allele through a spatially distributed population.

3.2. Maximum principle

According to the maximum principle, the solution of (1.5) remains nonnegative if the initial data $u_0(x) = u(x, 0)$ is non-negative, which is consistent with its use as a model of population or probability.

The maximum principle holds because if u first crosses from positive to negative values at time t_0 at the point x_0, and if $u(x, t)$ has a nondegenerate minimum at x_0, then $u_{xx}(x_0, t_0) > 0$. Hence, from (1.5), $u_t(x_0, t_0) > 0$, so u cannot evolve forward in time into the region $u < 0$. A more careful argument is required to deal with degenerate minima, and with boundaries, but the conclusion is the same [**18, 42**].

A similar argument shows that $u(x, t) \leq 1$ for all $t \geq 0$ if $u_0(x) \leq 1$.

Remark 1.3. A forth-order diffusion equation, such as

$$u_t = -u_{xxxx} + u(1-u),$$

does not satisfy a maximum principle, and it is possible for positive initial data to evolve into negative values.

3.3. Logistic equation

Spatially uniform solutions of (1.5) satisfy the logistic equation

$$u_t = ku(a-u). \tag{1.6}$$

This ODE has two equilibrium solutions at $u = 0$, $u = a$.

The solution $u = 0$ corresponds to a complete absence of the species, and is unstable. Small disturbances grow initially like $u_0 e^{kat}$. The solution $u = a$ corresponds to the maximum population that can be sustained by the available resources. It is globally asymptotically stable, meaning that any solution of (1.6) with a strictly positive initial value approaches a as $t \to \infty$.

Thus, the PDE (1.5) describes the evolution of a population that satisfies logistic dynamics at each point of space coupled with dispersal into regions of lower population.

3.4. Nondimensionalization

Before discussing (1.5) further, we simplify the equation by rescaling the variables to remove the constants. Let

$$u = U\bar{u}, \qquad x = L\bar{x}, \qquad t = T\bar{t}$$

where U, L, T are arbitrary positive constants. Then

$$\frac{\partial}{\partial x} = \frac{1}{L}\frac{\partial}{\partial \bar{x}}, \frac{\partial}{\partial t} = \frac{1}{T}\frac{\partial}{\partial \bar{t}}.$$

It follows that $\bar{u}\left(\bar{x}, \bar{t}\right)$ satisfies

$$\bar{u}_{\bar{t}} = \left(\frac{\nu T}{L^2}\right)\bar{u}_{\bar{x}\bar{x}} + (kTU)\,\bar{u}\left(\frac{a}{U} - \bar{u}\right).$$

Therefore, choosing

$$U = a, \qquad T = \frac{1}{ka}, \qquad L = \sqrt{\frac{\nu}{ka}}, \tag{1.7}$$

and dropping the bars, we find that $u(x,t)$ satisfies

$$u_t = u_{xx} + u(1-u). \tag{1.8}$$

Thus, in the absence of any other parameters, none of the coefficients in (1.5) are essential.

If we consider (1.5) on a finite domain of length ℓ, then the problem depends in an essential way on a dimensionless constant R, which we may write as

$$\mathrm{R} = \frac{ka\ell^2}{\nu}.$$

We could equivalently use $1/\mathrm{R}$ or $\sqrt{\mathrm{R}}$, or some other expression, instead of R. From (1.7), we have $\mathrm{R} = T_d/T_r$ where $T_r = T$ is a timescale for solutions of the reaction equation (1.6) to approach the equilibrium value a, and $T_d = \ell^2/\nu$ is a timescale for linear diffusion to significantly influence the entire length ℓ of the domain. The qualitative behavior of solutions depends on R.

When dimensionless parameters exist, we have a choice in how we define dimensionless variables. For example, on a finite domain, we could nondimensionalize as above, which would give (1.8) on a domain of length $\sqrt{R}$. Alternatively, we might prefer to use the length ℓ of the domain to nondimensionalize lengths. In that case, the nondimensionalized domain has length 1, and the nondimensionalized form of (1.5) is

$$u_t = \frac{1}{\mathrm{R}} u_{xx} + u\left(1-u\right).$$

We get a small, or large, dimensionless diffusivity if the diffusive timescale is large, or small, respectively, compared with the reaction time scale.

Somewhat less obviously, even on infinite domains additional lengthscales may be introduced into a problem by initial data

$$u(x,0) = u_0(x).$$

Using the variables (1.7), we get the nondimensionalized initial condition

$$\bar{u}\left(\bar{x},0\right) = \bar{u}_0\left(\bar{x}\right),$$

where

$$\bar{u}_0\left(\bar{x}\right) = \frac{1}{a} u_0\left(L\bar{x}\right).$$

Thus, for example, if u_0 has a typical amplitude a and varies over a typical lengthscale of ℓ, then we may write

$$u_0(x) = a\bar{f}\left(\frac{x}{\ell}\right)$$

where $\bar{f}$ is a dimensionless function. Then

$$\bar{u}_0\left(\bar{x}\right) = \bar{f}\left(\sqrt{\mathrm{R}}\bar{x}\right),$$

and the evolution of the solution depends upon whether the initial data varies rapidly, slowly, or on the same scale as the reaction-diffusion length scale L.

3.5. Traveling waves

One of the principal features of the KPP equation is the existence of traveling waves which describe the invasion of an unpopulated region (or a region whose population does not possess the favorable allele) from an adjacent populated region.

A traveling wave is a solution of the form

$$u(x,t) = f(x-ct) \tag{1.9}$$

where c is a constant wave speed. This solution consists of a fixed spatial profile that propagates with velocity c without changing its shape.

For definiteness we assume that $c > 0$. The case $c < 0$ can be reduced to this one by a reflection $x \mapsto -x$, which transforms a right-moving wave into a left-moving wave.

Use of (1.9) in (1.8) implies that $f(x)$ satisfies the ODE

$$f'' + cf' + f(1-f) = 0. \tag{1.10}$$

The equilibria of this ODE are $f = 0$, $f = 1$.

Note that (1.10) describes the spatial dynamics of traveling waves, whereas (1.6) describes the temporal dynamics of uniform solutions. Although these equations have the same equilibrium solutions, they are different ODEs (for example, one is second order, and the other first order) and the stability of their equilibrium solutions means different things.

The linearization of (1.10) at $f = 0$ is

$$f'' + cf' + f = 0.$$

The characteristic equation of this ODE is

$$\lambda^2 + c\lambda + 1 = 0$$

with roots

$$\lambda = \frac{1}{2}\left\{-c \pm \sqrt{c^2 - 4}\right\}.$$

Thus, the equilibrium $f = 0$ is a stable spiral point if $0 < c < 2$, a degenerate stable node if $c = 2$, and a stable node if $2 < c < \infty$.

The linearization of (1.10) at $f = 1$ is

$$f'' + cf' - f = 0.$$

The characteristic equation of this ODE is

$$\lambda^2 + c\lambda - 1 = 0$$

with roots

$$\lambda = \frac{1}{2}\left\{-c \pm \sqrt{c^2 + 4}\right\}.$$

Thus, the equilibrium $f = 1$ is a saddlepoint.

As we will show next, for any $2 \leq c < \infty$ there is a unique positive heteroclinic orbit $F(x)$ connecting the unstable saddle point at $f = 1$ to the stable equilibrium at $f = 0$, meaning that

$$F(x) \to 1 \quad \text{as } x \to -\infty; \qquad F(x) \to 0 \quad \text{as } x \to \infty.$$

These right-moving waves describe the invasion of the state $u = 0$ by the state $u = 1$. Reflecting $x \mapsto -x$, we get a corresponding family of left-moving traveling waves with $-\infty < c \leq -2$.

Since the traveling wave ODE (1.10) is autonomous, if $F(x)$ is a solution then so is $F(x - x_0)$ for any constant x_0. This solution has the same orbit as $F(x)$, and corresponds to a traveling wave of the same velocity that is translated by a constant distance x_0.

There is also a traveling wave solution for $0 < c < 2$ However, in that case the solution becomes negative near 0 since $f = 0$ is a spiral point. This solution is therefore not relevant to the biological application we have and mind. Moreover, by the maximum principle, it cannot arise from nonnegative initial data.

The traveling wave most relevant to the applications considered above is, perhaps, the positive one with the slowest speed ($c = 2$); this is the one that describes the mechanism of diffusion from the populated region into the unpopulated one, followed by logistic growth of the diffusive perturbation. The faster waves arise because of the growth of small, but nonzero, pre-existing perturbations of the unstable state $u = 0$ ahead of the wavefront.

The linear instability of the state $u = 0$ is arguably a defect of the model. If there were a threshold below which a small population died out, then this dependence of the wave speed on the decay rate of the initial data would not arise.

3.6. The existence of traveling waves

Let us discuss the existence of positive traveling waves in a little more detail.

If $c = 5/\sqrt{6}$, there is a simple explicit solution for the traveling wave [**1**]:

$$F(x) = \frac{1}{\left(1 + e^{x/\sqrt{6}}\right)^2}.$$

Although there is no similar explicit solution for general values of c, we can show the existence of traveling waves by a qualitative argument.

Writing (1.10) as a first order system of ODEs for (f, g), where $g = f'$, we get

$$\begin{aligned} f' &= g, \\ g' &= -f(1-f) - cg. \end{aligned} \tag{1.11}$$

For $c \geq 2$, we choose $0 < \beta \leq 1$ such that

$$\beta + \frac{1}{\beta} = c, \qquad \beta = \frac{1}{2}\left(c - \sqrt{c^2 - 4}\right).$$

Then, on the line $g = -\beta f$ with $0 < f \leq 1$, the trajectories of the system satisfy

$$\frac{dg}{df} = \frac{g'}{f'} = -c - \frac{f(1-f)}{g} = -c + \frac{1-f}{\beta} < -c + \frac{1}{\beta} = -\beta.$$

Since $f' < 0$ for $g < 0$, and $dg/df < -\beta$, the trajectories of the ODE enter the triangular region

$$D = \{(f, g) : 0 < f < 1, -\beta f < g < 0\}.$$

Moreover, since $g' < 0$ on $g = 0$ when $0 < f < 1$, and $f' < 0$ on $f = 1$ when $g < 0$, the region D is positively invariant (meaning that any trajectory that starts in the region remains in the region for all later times).

The linearization of the system (1.11) at the fixed point $(f, g) = (1, 0)$ is

$$\begin{pmatrix} f' \\ g' \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & -c \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix}.$$

The unstable manifold of $(1, 0)$, with corresponding eigenvalue

$$\lambda = \frac{1}{2}\left(-c + \sqrt{c^2 + 4}\right) > 0,$$

is in the direction

$$\vec{r} = \begin{pmatrix} -1 \\ -\lambda \end{pmatrix}.$$

The corresponding trajectory below the f-axis must remain in D, and since D contains no other fixed points or limit cycles, it must approach the fixed point $(0, 0)$ as $x \to \infty$.

Thus, a nonnegative traveling wave connecting $f = 1$ to $f = 0$ exists for every $c \geq 2$.

3.7. The initial value problem

Consider the following initial value problem for the KPP equation

$$\begin{aligned} &u_t = u_{xx} + u(1-u), \\ &u(x, 0) = u_0(x), \\ &u(x, t) \to 1 \text{ as } x \to -\infty, \\ &u(x, t) \to 0 \text{ as } x \to \infty. \end{aligned}$$

Kolmogorov, Petrovsky and Piskunov proved that if $0 \leq u_0(x) \leq 1$ is any initial data that is exactly equal to 1 for all sufficiently large negative x, and exactly equal to 0 for all sufficiently large positive x, then the solution approaches the traveling wave with $c = 2$ as $t \to \infty$.

This result is sensitive to a change in the spatial decay rate of the initial data into the unstable state $u = 0$. Specifically, suppose that

$$u_0(x) \sim Ce^{-\beta x}$$

as $x \to \infty$, where β is some positive constant (and C is nonzero). If $\beta \geq 1$, then the solution approaches a traveling wave of speed 2; but if $0 < \beta < 1$, meaning that the initial data decays more slowly, then the solution approaches a traveling wave of speed

$$c(\beta) = \beta + \frac{1}{\beta}.$$

This is the wave speed of the traveling wave solution of (1.10) that decays to $f = 0$ at the rate $f \sim Ce^{-\beta x}$.

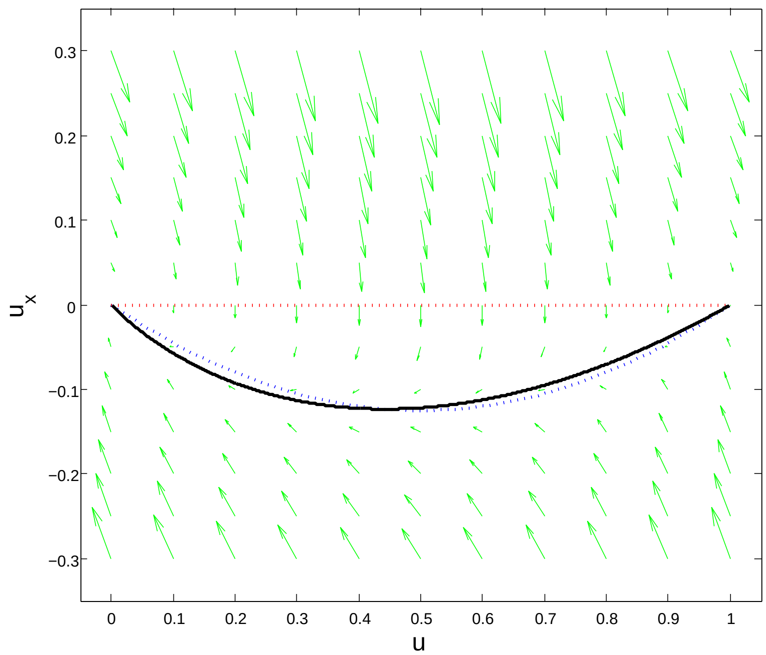

FIGURE 1. The phase plane for the KPP traveling wave, showing the heteroclinic orbit connecting $(1, 0)$ to $(0, 0)$ (courtesy of Tim Lewis).

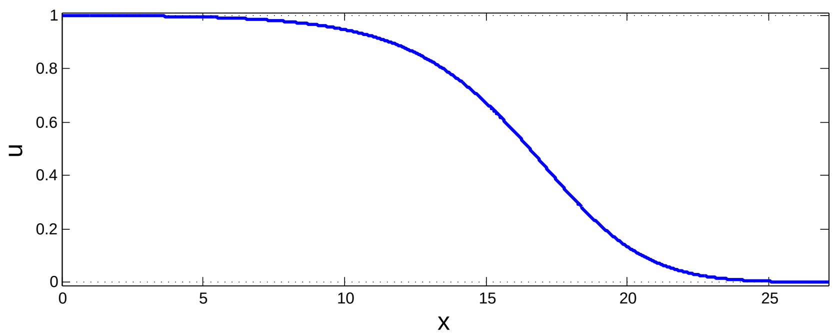

FIGURE 2. The spatial profile of the traveling wave.