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Abstract. We obtain a novel infinite parametric class of exact, stable travelling-wave solutions of the one-component, one-dimensional reaction diffusion equation by means of an inverse method. A number of explicit examples are worked out in terms of elementary functions. Some special cases of two-component, travelling-wave, reaction–diffusion problems can be reduced to the one-component case and thus solved by our method.

1. Introduction

For many years mathematical biology and chemistry books have quoted the Fisher [1] equation (1) as a more or less idealized model in genetics of populations, chemical kinetics, etc:

$$\partial c(x, t)/\partial t = D\partial^2 c(x, t)/\partial x^2 + f(c(x, t)). \tag{1}$$

The term $f(c)$ characterizes the rate of variation of concentration in the absence of diffusion. Kolmogorov *et al* [2] analysed the special case in which $f(c)$ has roots at $c = 0, 1$ and is monotonically convex with a step-like initial condition. Recently, Freidlin [3], using the Feynman–Kac integral solution for Cauchy's problem, provided a general wave solution of (1) restricted to slow reaction rates ($f(c) \sim 0$). Unlike [3], we pursue here an inverse solution for those cases in which the reaction rate is a 'strong' function of the local change in concentration. We provide an algorithm for some concrete problems. An example of this would be the spreading of an excitation in a medium [3] or the diffusion of reacting macromolecules in a medium (involving solvent) in which a localized reversible reaction occurs between the macromolecules. We obtain analytic expressions for the wavefront in the concentration, $c(x + vt)$, and for the reaction rate as a function of the concentration, $f(c)$. We discuss the stability of the wave solutions, and construct parametric classes of them and consider generalizations to some multi-component systems. Our implicit solutions are expressible in quadratures and in a number of examples, involve only elementary transcendental functions. The propagation velocities can be either positive or negative, depending on the boundary condition which will be subsequently introduced.

2. Basic solution

Consider a wave solution, of a leftward travelling wave with $v > 0$:

$$c(x, t) = \phi(\xi) \qquad \xi = x + vt. \tag{2}$$

The origin of the pattern is most simply fixed by requiring

$$\phi''(0) = 0. \tag{3}$$

Equation (1) now becomes

$$v\phi'(\xi) = D\phi''(\xi) + f(\phi(\xi)). \tag{4}$$

For a wave solution, say from zero concentration (this level is merely a convenience) to a saturating concentration c_M, we will want to have

$$\phi(\xi) \to 0, \phi'(\xi) \to 0 \qquad \text{as } \xi \to -\infty$$
$$\phi(\xi) \to c_M, \phi'(\xi) \to 0 \qquad \text{as } \xi \to \infty. \tag{5}$$

Since (4) is autonomous, one can carry out a standard degree-lowering transformation by switching from the variables $\phi(\xi)$ and ξ to $\Psi(\phi)$ and ϕ where

$$\Psi(\phi(\xi)) = \phi'(\xi). \tag{6}$$

Doing so, (4) reduces to

$$v\Psi(\phi) = D\Psi(\phi)\Psi'(\phi) + f(\phi) \tag{7}$$

with associated conditions

$$\Psi(\phi) \to 0 \qquad \text{as } \phi \to 0 \text{ or } \phi \to c_M. \tag{8}$$

It will also be convenient to choose that solution of (3) such that the absolute maximum of ϕ is at $\xi = 0$; the corresponding value

$$\Psi_0 = \Psi(\phi(0)) \tag{9}$$

will serve as a reference.

The equation (7) has known solutions [4] for special functions $f(\phi)$, but not with boundary conditions (8). One not very informative way of producing solutions to (4) is by total inversion of the problem: choose a solution $\phi(\xi)$ and ask for that f which produces it; a similar procedure is available for (8). But one can instead go only part way towards triviality by supposing that $f(\phi)$ is known as a function of Ψ:

$$f(\phi) = R(\Psi(\phi)) \tag{10}$$

and afterwards find out what function f really is, and what concentration profile it produces. Hence we now have

$$v\Psi(\phi) = D\Psi(\phi)\Psi'(\phi) + R(\Psi(\phi)) \tag{11}$$

which is directly solvable by reversing the roles of the variables Ψ and ϕ; i.e. write $\phi = c(\Psi)$, so that (11) becomes

$$c'(\Psi) = D\Psi/(v\Psi - R(\Psi)). \tag{12}$$

Setting

$$G(\Psi) = R(\Psi)/v\Psi \tag{13}$$

puts (12) in the form

$$c'(\Psi) = D/v(1 - G(\Psi)) \tag{14}$$

and the boundary conditions (8) then become

$$c(0) = 0 \text{ or } c_{\text{M}}. \tag{15}$$

Hence $G(\Psi)$ must be at least a two-valued function.

A non-dimensional form of (14), (15) is of course to be preferred. We set

$$\Psi^* = \Psi/\Psi_0 \qquad v^* = c_{\text{M}}v/D\Psi_0 \qquad G^*(\Psi^*) = G(\Psi)$$

$$c^*(\Psi^*) = c(\Psi)/c_{\text{M}} \tag{16}$$

so that now on the space $0 \leqslant \Psi^* \leqslant 1$ we have

$$v^* \, dc^*/d\Psi^* = 1/(1 - G^*(\Psi^*))$$

$$c^*(0) = 0 \text{ or } 1 \qquad \text{with } c^*(1) \text{ single-valued.} \tag{17}$$

A simple example is instructive. Choose the familiar tanh profile, normalizing so that $c_{\text{M}} = 1$ and $\Psi_0 = 1$ (hence $c^* = c$, $\Psi^* = \Psi$, $G^* = G$):

$$\phi(\xi) = \tfrac{1}{2}[1 + \tanh(2\xi)] \tag{18}$$

then $\Psi(\xi) = \mathrm{sech}^2(2\xi)$, so

$$\phi = c(\Psi) = \tfrac{1}{2}(1 \pm \sqrt{1 - \Psi}) \tag{19}$$

hence $c'(\Psi) = \mp 1/(4\sqrt{1 - \Psi})$, and

$$G(\Psi) = 1 \pm (4/v^*)\sqrt{1 - \Psi}. \tag{20}$$

This means that $R(\Psi) = v^*\Psi[1 \pm (4/v^*)\sqrt{1 - \Psi}]$, but $\Psi = 4\phi(1 - \phi)$ and so, choosing the correct sign,

$$f(c) = 4v^*c(1 - c) + 16Dc(1 - c)(2c - 1). \tag{21}$$

The two-valuedness of G is of course just a reflection of that of $\phi = c(\Psi)$.

3. Local stability

We now have a routine for producing reaction-rate profile pairs at a given propagation velocity v. But are these stable? Will they actually be achieved? These questions are not quite the same. One knows (mainly from the Fisher–Kolmogorov example) that if (5) is satisfied initially in time, then only a single characteristic velocity will asymptotically propagate. Computer simulations on large finite systems come to the same conclusion. However, there is normally a whole band of velocities for which the solution is locally stable, i.e. to a linearized perturbation and hence to a superposition of local perturbations. Analysis of the latter effect does not require the analytic machinery that the former does, and so let us see what happens in our solution. We must be aware, of course, that changing v also changes our reaction function, so that when we assess the stability of a given parameterization, the band of v we may encounter is not the one ordinarily referred to.

To assess the stability of a given solution $\phi_0(\xi)$ to (1) we, as usual, set

$$c(x, t) = \phi_0(x + vt) + e^{-\lambda' t}\Delta(x + vt) \tag{22}$$

where Δ is infinitesimal, obtaining

$$-D\Delta''(\xi) + v\Delta'(\xi) - f'(\phi_0(\xi))\Delta(\xi) = \lambda\Delta(\xi)$$

$$\Delta(-\infty) = 0 \qquad \Delta(\infty) \text{ finite.} \tag{23}$$

Hence with $y(\xi) = \exp[-(v/2D)\xi]\Delta(\xi)$

$$-Dy''(\xi) + (v^2/4D - f'(\phi_0(\xi)))y(\xi) = \lambda y(\xi) \qquad y(\pm\infty) = 0. \tag{24}$$

Stability requires that all $\lambda > 0$. Now $R = v\Psi - D\Psi\Psi'$, so

$$\mathrm{d}R/\mathrm{d}\phi = v\phi''(\xi)/\phi'(\xi) - D\phi'''(\xi)/\phi'(\xi)$$

and (24) becomes

$$-y''(\xi) + \tfrac{1}{4}(v/D)^2 y(\xi) + (\phi'''(\xi) - v\phi''(\xi)/D)y(\xi)/\phi'(\xi) = \lambda y(\xi)/D. \tag{25}$$

For large v/D, clearly $\lambda > 0$; for $v = 0$, $\lambda = 0$ occurs (with $y = \phi_0'$) and so $\lambda < 0$ is possible. Hence, in general one expects a minimum velocity $v_{\min}$, above which local stability applies.

4. A survey of solutions

Let us look at a few more examples. Instead of (18), choose

$$\phi(\xi) = \tfrac{1}{2} + (1/\pi)\tan^{-1}(\pi\xi). \tag{26}$$

Then $\Psi(\xi) = 1/(1 + \pi^2\xi^2)$, so

$$\phi = c(\Psi) = \tfrac{1}{2} \pm (1/\pi)\tan^{-1}(\sqrt{1/\Psi - 1}). \tag{27}$$

Hence $c'(\Psi) = \mp(1/2\pi)/\sqrt{(1/\Psi) - 1}$ and

$$G(\Psi) = 1 \pm 2\pi\sqrt{(1 - \Psi)/\Psi} \tag{28}$$

surprisingly similar to (20).
     Another example is

$$\phi(\xi) = (2/\pi)\tan^{-1}(e^{\pi\xi}) \tag{29}$$

so that $\Psi(\xi) = \operatorname{sech}(\pi\xi)$, and

$$\phi = c(\Psi) = \pm(1/\pi)\sin^{-1}(\Psi). \tag{30}$$

Thus, $c'(\Psi) = \pm(1/\pi)/\sqrt{1 - \Psi^2}$, and

$$G(\Psi) = 1 \pm \pi\sqrt{1 - \Psi^2} \tag{31}$$

also very similar to (20).
     It is not necessary to use analytic functions. Suppose

$$\phi(\xi) = \tfrac{1}{2}[1 + (1 - e^{-2|\xi|})\operatorname{sgn}(\xi)]. \tag{32}$$

Now $\Psi(\xi) = e^{-2|\xi|}$, and

$$\phi = c(\Psi) = \tfrac{1}{2}[1 \pm (1 - \Psi)]. \tag{33}$$

Hence $c'(\Psi) = \tfrac{1}{2}$ and

$$G(\Psi) = -1, 3. \tag{34}$$

The associated reaction rates can routinely be derived, but we will do this in a more general context.

5. Construction of parametric classes

We now implement the inverse strategy. This calls for representing $G^*(\Psi^*)$ of (17) parametrically, solving for the profile—which incidentally fixes v^*—and also for the reaction rate. Fitting the latter to input information then allows determination of the consequent profile.

It is clear from the examples of section 4 that an appropriate form is

$$G^*(\Psi^*) = 1 \pm g(\Psi^*)\sqrt{1 - \Psi^*}/2 \tag{35}$$

for a suitable single-valued g, so that in (17)

$$v^* \partial c^*/\partial \Psi^* = \pm (2\sqrt{1 - \Psi^*}\, g(\Psi^*))^{-1}. \tag{36}$$

The form (35) will produce a symmetric profile; for asymmetry, one would, of course use $g_1/2$ and $-g_2/2$. If we set

$$\psi = \sqrt{1 - \Psi^*} \tag{37}$$

(36) simplifies to

$$v^* \partial c^*/\partial \psi = \pm 1/g(1 - \psi^2). \tag{38}$$

In terms of the new variable ψ, we have the conditions

$$c^*(0) \text{ is single-valued} \qquad c^*(1) = 0 \text{ or } 1. \tag{39}$$

By integrating (38), we see at once that $c^*(0) = \frac{1}{2}$ and that

$$v^* = 2 \int_0^1 \frac{\mathrm{d}t}{g(1 - t^2)} \qquad c^*(\psi) = \frac{1}{2} \pm \frac{1}{v^*} \int_0^\psi \frac{\mathrm{d}t}{g(1 - t^2)}. \tag{40}$$

Suppose, for example, that $g(\Psi^*) = a(1 + b\Psi^*)$, $0 < b < 1$, then

$$v^* = 2/[a\sqrt{b(1+b)}]\tanh^{-1}\sqrt{b/1+b} \tag{41}$$

$$c^*(\psi) = \frac{1}{2} \pm \frac{1}{2}\tanh^{-1}\sqrt{b\psi/(1+b)}/\tanh^{-1}\sqrt{b/(1+b)}$$
$$= \frac{1}{2} \pm \frac{1}{2}\tanh^{-1}\sqrt{b(1-\Psi^*)/(1+b)}/\tanh^{-1}\sqrt{b/(1+b)}. \tag{42}$$

Hence

$$\Psi^* = 1 - [(1+b)/b]\tanh^2[(2c^* - 1)\tanh^{-1}\sqrt{b/(1+b)}]. \tag{43}$$

On the one hand, with $c^*(\psi^*) = \phi^*(\xi)$ we have

$$\Psi^* = \mathrm{d}\phi^*/\mathrm{d}\xi$$

so that

$$\mathrm{d}\xi = \mathrm{d}\phi^*/\{1 - [(1+b)/b]\tanh^2[(2\phi^* - 1)\tanh^{-1}\sqrt{b/(1+b)}]\} \tag{44}$$

giving rise to the profile in the form

$$\xi = -b(2\phi^* - 1)/2 + \sqrt{b(1+b)}\tanh^{-1}\{\sqrt{(1+b)/b}\tanh[(2\phi^* - 1)$$
$$\times \tanh^{-1}\sqrt{b/(1+b)}]\}/2\tanh^{-1}\sqrt{b/(1+b)}. \tag{45}$$

On the other hand, $f(c^*) = v^*\Psi^*G(\Psi^*)$ produces the reaction rate

$$f(c^*) = 2\tanh^{-1}\sqrt{b/(1+b)}\{b + 1 - (1 + 1/b)$$
$$\times \sinh^2[(2c^* - 1)\tanh^{-1}\sqrt{b/(1+b)}]/\{\sqrt{b(1+b)}$$
$$\times \cosh^4[(2c^* - 1)\tanh^{-1}\sqrt{b/(1+b)}]\} \tag{46}$$

to which input data is to be fitted.

Another accessible example is

$$g(\Psi^*) = a\sqrt{1 + b\Psi^*} \qquad b > 0 \tag{47}$$

then, following the steps above:

$$v^* = 2\sin^{-1}\sqrt{b/(1+b)}/(a\sqrt{1+b}) \tag{48}$$

$$c^* = \tfrac{1}{2} \pm \tfrac{1}{2}\sin^{-1}\sqrt{(b/1+b)(1-\Psi^*)}/\sin^{-1}\sqrt{b/(1+b)}$$

$$\Psi^* = 1 - [(1+b)/b]\sin^2[(2c^*-1)\sin^{-1}\sqrt{b/(1+b)}]$$

giving rise to the profile and the reaction rate in the form

$$\xi = [(1+b)/4]\ln\left(\frac{\sin[\sin^{-1}\sqrt{b/1+b}(2\phi^*-1)] + \sqrt{b}\cos[\sin^{-1}\sqrt{b/(1+b)}(2\phi^*-1)]}{\sin[\sin^{-1}\sqrt{b/(1+b)}(2\phi^*-1)] - \sqrt{b}\cos[\sin^{-1}\sqrt{b/1+b}(2\phi^*-1)]}\right) \tag{49}$$

$$f(c^*) = 2\sin^{-1}\sqrt{b/(1+b)}\{\cos^2(\sin^{-1}\sqrt{b/(1+b)}(2c^{*-1})](b+1) - 1\}$$
$$\times \{1 - \sin^2[\sin^{-1}\sqrt{b/(1+b)}(2c^*-1)]\}.$$

6. Multicomponent systems

There are circumstances under which multicomponent systems can be reduced to equivalent one-component form and hence can be tackled by the above technique. The most realistic case is that in which all components but one diffuse very rapidly, and hence are present uniformly in the system. Consider for example the two-component case

$$\dot{c}_1 = D_1 c_1'' + f_1(c_1, c_2) \tag{50a}$$

$$\dot{c}_2 = d_2 c_2'' + f_2(c_2, c_2) \tag{50b}$$

and suppose that $D_2 \to \infty$, so that in a bounded system

$$c_2(x, t) = \gamma(t). \tag{51}$$

Averaging (50b) over the system space, we have

$$\gamma(t) = \langle f_2(c_1(x, t), \gamma(t)) \rangle_x \tag{52}$$

which must vanish in steady flow. But for wave propagation

$$c(x, t) = \phi(\xi) \qquad \xi = x + vt. \tag{53}$$

So we require the constant γ to satisfy

$$\langle f_2(\phi(\xi), \gamma) \rangle_\xi = 0 \tag{54}$$

which, since $f_2 = 0$ in either high or low concentration plateau regions, is best written as

$$\int_{-\infty}^{\infty} f_2(\phi(\xi), \gamma)\, d\xi = 0. \tag{55}$$

It is (55), coupled with (50a) in the form

$$v\phi'(\xi) = D_1\phi''(\xi) + f_1(\phi(\xi), \gamma) \tag{56}$$

which constitutes the self-consistent set to be solved. The procedure, following section 5, is clear but certainly depends upon the class of reaction rates to be examined. It may be noted in passing that the self-consistent determination (55) of γ takes the procedure out of the realm of the purely mathematical models considered by Lefevre *et al* [5, 6]. However, it should also be noted that the solution (50*a*), (55) is strictly valid only if $\gamma(t)$ varies slowly—behaves as a constant—on the timescale established by the velocity v and the width of the concentration profile.

We mention another special case, alluded to in the introduction, in which two coupled reaction-diffusion equations possess travelling-wave solutions of the kind we have described. Consider a large macromolecule which has a small site which can exist in two states: 1, 2. The diffusion coefficient of both macromolecular species in some medium can then be taken to be identical: $D_1 = D_2 = D$, determined only by the overall size and shape of the molecule. Denoting by $f_{12}(c_1, c_2)$ the rate of conversion of species 1 into species 2, the basic equations in $y = x + vt$ to be solved are

$$v \, \mathrm{d}c_1/\mathrm{d}y = f_{12}(c_1, c_2) + D \, \mathrm{d}^2c_1/\mathrm{d}y^2$$
$$v \, \mathrm{d}c_2/\mathrm{d}y = -f_{12}(c_1, c_2) + D \, \mathrm{d}^2c_2/\mathrm{d}y^2$$

(57)

with boundary conditions on c_2 such that $c_1(y) + c_2(y) = c_0$, a constant (i.e. $c_1(0) + c_2(0) = c_1(\infty) + c_2(\infty) = c_0$). Then (57) reduces to (2) with $f_{12}(c_1, c_0 - c_1) = f(c_1)$.

7. Concluding remarks

It has already been pointed out [7] that the Fisher-Kolmogorov equation and its generalizations are idealized and simplified models of some qualitative features of real genetic and chemical processes rather than a strict quantitative model of a specific experimental instance. This is of course true of our examples. A computerized literature search shows no chemical system which can be quantitatively analysed by this theory. Nevertheless it is still interesting to study the relation between the qualitative form of the reaction rate and the behaviour of the solution of (1) particularly if this can be done fairly explicitly with our class of inverse solutions.

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