Speed of fronts of generalized reaction-diffusion equations

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Recent work on generalized diffusion equations has given analytical and numerical evidence that, as in the standard reaction-diffusion equation, most initial conditions evolve into a traveling wave which corresponds to a minimum speed front joining a stable to an unstable state. We show that this minimal speed derives from a variational principle; from this we recover linear constraints on the speed (the linear marginal stability value) and provide upper and lower bounds on the speed. This enables us to characterize the functions for which linear marginal stability holds and also to provide a tool to calculate the speed when the marginal value does not predict its correct value. [S1063-651X(98)09906-1]

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Different problems may be described in terms of the reaction-diffusion equation $u_t = u_{xx} + f(u)$, where f is a nonlinear term with at least two equilibrium points. It has been established rigorously [1] that sufficiently localized initial conditions evolve asymptotically into a traveling monotonic wave front $u(x-ct)$ joining two equilibrium states. For simplicity we will consider reaction terms $f>0$ which vanish at $u=0$ and at $u=1$. There is a wide class of reaction terms $f(u)$ for which this asymptotic speed is given by [2] the Kolmogorv-Petrovskii-Piskunov (KPP) value $c_{KPP} = 2\sqrt{f'(0)}$. This is the minimal value of the speed that follows from a linear analysis at the equilibrium points. The extension of this behavior to pattern-forming systems is called the [3] marginal stability hypothesis. For other reaction terms this linear or c_{KPP} value represents a lower bound to the speed. There exist local [4] and global [5,6] variational principles that enable one to determine the speed for arbitrary reaction terms $f(u)$, as well as methods based on approximate solutions of the differential equation itself [7,8]. While all the above results have been established rigorously, other problems are described by other types of reaction-diffusion equations in which nonlinearities may appear on derivative terms. Generalized diffusion equations of the form $u_t = u_{xx} + F(u_x, u)$ and the stability of its traveling fronts have been studied [9,10]. While the stability of its traveling waves has been established, the problem of determining which of the possible traveling waves will be the asymptotic state has not been clarified in general. In recent work [11] one such type of generalized reaction diffusion equation, namely,

$$\phi_t = \phi_{xx} + \frac{m}{1-\phi}\phi_x^2 + f(\phi), \tag{1}$$

with $f(\phi) = \phi(1-\phi)$, has been considered. This equation has traveling wave fronts $\phi(x-ct)$ joining the stable state $\phi=1$ to $\phi=0$. Exact analytical solutions to the partial differential equation (PDE) have been found [11] for the case $m=2$, which show explicitly that in the time evolution the front of minimal speed is selected. Numerical integrations for other values of m and for reaction terms of the form $f(\phi) = (1-\phi)[1-(1-\phi)^\beta]$ support this conclusion. For these reaction terms it is found that the system evolves into the front of minimal speed which, for these reaction terms, is the so called marginal stability value obtained from linear considerations at the equilibrium points. As it occurs in the usual reaction-diffusion equation, the selected speed is not always the linear marginal value [12]; for other reaction terms it is greater than the linear value and no analytic procedure to calculate the speed has been given for these generalized reaction-diffusion equations. In this work we provide such a method and obtain upper bounds which enable us to characterize the reaction terms for which marginal stability holds. While for concreteness we present results for Eq. (1), the method can be extended to many other types of generalized reaction-diffusion equations. We assume then, based on the evidence presented in [11], that, for general reaction terms $f(\phi)$, many initial conditions for Eq. (1) evolve into the traveling front $\phi(x-ct)$ of minimal speed. We will show that the minimal speed is given by

$$c = \max_g \frac{2\int_0^1 \sqrt{fg[mg/(1-\phi) - g']}\,d\phi}{\int_0^1 g(\phi)\,d\phi} \tag{2}$$

for a certain class of trial functions g. (Rigorously, the speed is the maximum when $c > c_L$ defined below. It is the supremum when $c = c_L$.) From here it will follow that

$$c_L \leq c \leq 2\sqrt{\sup_\phi \left(f'(\phi) + \frac{m f(\phi)}{1-\phi} \right)}, \tag{3}$$

where c_L is the marginal stability value [11],

$$c_L = \max(2\sqrt{f'(0)}, 2\sqrt{|f'(1)|(m-1)}).$$

From the variational expression (2) one may obtain the value of the speed with any desired accuracy, and the inequality (3) enables us to characterize the functions for which the speed is the linear marginal stability value. We now show the calculations.

The front is a solution of

$$\phi_{zz} + c\phi_z + \frac{m}{1-\phi}\phi_z^2 + f(\phi) = 0,$$

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where $z=x-ct$ with boundary conditions $\lim\phi_{z\to-\infty}=1$ and $\lim\phi_{z\to\infty}=0$ and $\phi_z<0$ in (0,1). ϕ_z vanishes when $z\to\pm\infty$. Following the usual procedure, for monotonic fronts it is convenient to work in phase space. Defining $p(\phi)=-\phi_z$ we have that monotonic fronts are solutions of

$$p\frac{dp}{d\phi}-cp+\frac{m}{1-\phi}p^2+f(\phi)=0, \tag{4}$$

with

$$p(0)=p(1)=0, \quad p>0 \quad \text{in } (0,1).$$

Since we are assuming $f(\phi)>0$, the simplest method is as given in [12,5] with appropriate modifications. Let $g(\phi)$ be an arbitrary positive function; multiplying Eq. (4) by g/p and integrating we obtain, after integration by parts,

$$c\int_0^1 g(\phi)d\phi=\int_0^1 d\phi\left[\frac{gf}{p}+p\left(\frac{mg}{1-\phi}-g'\right)\right].$$

Choosing g such that

$$\frac{mg}{(1-\phi)}-g'>0, \tag{5}$$

we have that, since f, g, and p are positive,

$$F(p)\equiv\frac{gf}{p}+p\left(\frac{mg}{1-\phi}-g'\right)\geqslant 2\sqrt{fg\left(\frac{mg}{1-\phi}-g'\right)}$$

and therefore

$$c\geqslant\frac{2\int_0^1\sqrt{fg[mg/(1-\phi)-g']}d\phi}{\int_0^1 g(\phi)d\phi}, \tag{6}$$

where the equal sign holds for $g=\hat{g}$ such that

$$\frac{\hat{g}'}{\hat{g}}=\frac{p'}{p}-\frac{c}{p}+\frac{2m}{1-\phi}.$$

This can be solved for $\hat{g}$ in terms of p and ϕ. The solution is given by

$$\hat{g}=\frac{p}{(1-\phi)^{2m}}\exp\left(-\int_{\phi_0}^{\phi}\frac{c}{p}d\phi'\right).$$

A careful analysis (which we do not spell out) of the singularities at $\phi=0$ and at $\phi=1$ shows that the integral of $\hat{g}$ exists whenever $c>c_L$ which proves our main result, Eq. (2). The above expression (6) can be used to calculate the asymptotic speed of the front for arbitrary reaction terms f, provided that the hypothesis that a minimal speed front is selected remains true.

At this point it is convenient to recall explicitly the extended marginal stability result obtained in [11] for some reaction terms. In contrast with the usual case, they observe that the analysis of both equilibrium points imposes constraints on the allowed value of the speed. Their generalized marginal stability hypothesis is then that the value of the speed is the greater of the constraints. For the case $f(\phi)=\phi(1-\phi)$ the linear value of the speed is $c_L=\max(2,2\sqrt{m-1})$; for a different reaction term, namely, $f(\phi)=(1-\phi)[1-(1-\phi)^{\beta}]$, they obtain $c_L=\max(2\sqrt{\beta},2\sqrt{m-1})$. We wish to show that the variational expression (6) for c yields as a lower bound the linear marginal values and at the same time [12] provides a criterion for its validity. We will show that the marginal stability value c_L for the speed follows directly from the variational expression (6). And we shall also show that the variational principle enables one to obtain an upper bound on the speed, namely, analogous to Aronson and Weinberger's result $2\sqrt{\sup(f(u)/u)}$, which permits the characterization of functions for which the linear marginal stability value holds. To obtain the constraint imposed by the behavior of the front at the stable fixed point $\phi=1$ consider the sequence of trial functions $g_{1\alpha}=(1-\phi)^{\alpha-1}$ in the limit $\alpha\to 0$. Evaluating the bound with $g_{1\alpha}$ we obtain

$$c\geqslant 2\alpha\sqrt{m+\alpha-1}\int_0^1\sqrt{f(\phi)}(1-\phi)^{\alpha-3/2}d\phi.$$

In the limit $\alpha\to 0$ the integrand is divergent at $\phi=1$, and as a result of the overall factor of α, only the singular point will contribute in the limit. The surviving term is then

$$c\geqslant 2\alpha\sqrt{m+\alpha-1}\int_{1-\epsilon}^1\sqrt{f(\phi)}(1-\phi)^{\alpha-3/2}d\phi.$$

We may now expand $f(\phi)$ in a Taylor series near 1. Here only the leading term in the expansion will contribute as the others will be regular when $\alpha\to 0$. We obtain then that the only contribution in the limit is

$$c\geqslant 2\alpha\sqrt{|f'(1)|(m+\alpha-1)}\int_{1-\epsilon}^1(1-\phi)^{\alpha-1}d\phi$$
$$=2\alpha\sqrt{|f'(1)|(m+\alpha-1)}\frac{\epsilon^{\alpha}}{\alpha},$$

which in the limit $\alpha\to 0$ is

$$c\geqslant 2\sqrt{|f'(1)|(m-1)}.$$

Notice that there is no inconsistency with the classical case $m=0$ since the trial function is only admissible [i.e., satisfies Eq. (5)] for $m>1$. Thus, the above result cannot be evaluated at $m=0$.

To obtain the bound that follows from the behavior of the front at the unstable point $\phi=0$ consider the sequence of trial functions $g_{2\alpha}=\phi^{\alpha-1}$ in the limit $\alpha\to 0$. Evaluating the bound with $g_{2\alpha}$ we obtain

$$c\geqslant 2\alpha\int_0^1\phi^{\alpha-3/2}\sqrt{f(\phi)\left(\frac{m\phi}{1-\phi}-(\alpha-1)\right)}\,d\phi.$$

Now, in the limit $\alpha \to 0$ the integrand is divergent at $\phi=0$ and, again, as a result of the overall factor of α, only the singular point will contribute in the limit. The only surviving term is

$$c \geqslant 2\alpha \int_0^\epsilon \phi^{\alpha-3/2} \sqrt{f(\phi)\left(\frac{m\phi}{1-\phi}-(\alpha-1)\right)}\, d\phi.$$

Expanding the term under the root in a Taylor series we find that only the leading term gives a singular contribution, that is,

$$c \geqslant 2\alpha\sqrt{f'(0)(1-\alpha)}\int_0^\epsilon \phi^{\alpha-1} d\phi = 2\alpha\sqrt{f'(0)(1-\alpha)}\frac{\epsilon^\alpha}{\alpha},$$

which in the limit $\alpha \to 0$ is

$$c \geqslant 2\sqrt{f'(0)}.$$

To sum up, the speed is bounded below by Eq. (6), where g is a positive trial function that satisfies condition (5). With two properly chosen trial functions we have obtained two lower bounds; obviously the greater of them is the best bound. The trial functions have been chosen to extract the behavior at the edges of the front and correspond to the so-called linear marginal stability value. We now proceed to obtain an upper bound for the speed. We shall need the inequality [13]

$$\sqrt{\frac{\int_0^1 \alpha(x)\mu(x)d\,x}{\int_0^1 \mu(x)d\,x}} \geqslant \int_0^1 \frac{\sqrt{\alpha(x)}\mu(x)d\,x}{\int_0^1 \mu(x)d\,x},$$

where $\mu(x) > 0$ and $\alpha(x) \geqslant 0$. (This is a particular case of Jensen's inequality.) Call $h \equiv 2mg/(1-\phi) - g'$ which is positive by construction. We have then, using the inequality above (with $\alpha = fh/g$ and $\mu = g$), that

$$c = \max_g 2\frac{\int_0^1 \sqrt{fgh}\, d\phi}{\int_0^1 g\, d\phi} = \max_g 2\frac{\int_0^1 \sqrt{(fh/g)}\, g\, d\phi}{\int_0^1 g\, d\phi}$$

$$\leqslant 2\max_g \sqrt{\frac{\int_0^1 (fh/g)\, g\, d\phi}{\int_0^1 g\, d\phi}} = 2\max_g \sqrt{\frac{\int_0^1 fh\, d\phi}{\int_0^1 g\, d\phi}}. \tag{7}$$

Now observe that

$$\int_0^1 fh d\phi = \int_0^1 f\left(\frac{mg}{1-\phi}-g'\right) d\phi$$

$$= -\int_0^1 f(1-\phi)^{-m}\frac{d}{d\phi}[(1-\phi)^m g]\, d\phi,$$

and integrating by parts we have that

$$\int_0^1 fh\, d\phi = \int_0^1 (1-\phi)^m g \frac{d}{d\phi}[f(1-\phi)^{-m}]\, d\phi$$

$$= \int_0^1 g\left[f' + \frac{mf}{1-\phi}\right] d\phi$$

$$\leqslant \sup_\phi\left[f' + \frac{mf}{1-\phi}\right]\int_0^1 g d\phi;$$

so we finally have

$$c = \max_g 2\frac{\int_0^1 \sqrt{fgh}\, d\phi}{\int_0^1 g\, d\phi} \leqslant 2\max_g \sqrt{\frac{\int_0^1 fh\, d\phi}{\int_0^1 g\, d\phi}}$$

$$\leqslant 2\sqrt{\sup_\phi\left[f' + \frac{mf}{1-\phi}\right]},$$

which was the desired result.

As an example let $f(\phi) = \phi(1-\phi)$. We obtain $f' + mf/(1-\phi) = 1 + (m-2)\phi$ and its maximum occurs at $\phi = 0$ and is 1 when $m < 2$ whereas when $m > 2$ the maximum occurs at $\phi = 1$ and is $m-1$; that is, we obtain that the upper and lower bounds in Eq. (3) coincide and the speed can be predicted without uncertainty. The speed may, for some reaction terms, be larger and can be calculated from Eq. (6).

Although we have presented results for the generalized reaction-diffusion equation (1), the method is not peculiar to this problem; a similar approach will be useful for other generalized reaction-diffusion equations which select a minimal speed front. Here we have relied on numerical and analytical evidence that such a front is selected; a full proof remains to be given.

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