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Series solution of nonlinear coupled reaction-diffusion equations

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Abstract. A nonlinear set of two coupled reaction-diffusion equations is investigated analytically to obtain travelling wave solutions. First, the series method of Hereman *et al.*, involving powers of decaying exponentials, is used to determine the width and the velocity of those waves. Further, to get a suitable analytical expression for them, another power series is introduced for which now a tanh function acts as new variable. As a result, recursion relations can be set up. Keeping only the lowest order terms, neglecting coefficients of higher order, we find solutions which correspond with earlier numerical calculations.

We study a set of two nonlinear dynamical equations, which describe reaction and diffusion in simple autocatalytic systems with linear decay. It was shown numerically that in such systems travelling wave solutions could exist (Merkin and Needham 1989), for certain values of the linear decay parameter. This set is written as:

$$\frac{\partial \alpha}{\partial t} = \frac{\partial^2 \alpha}{\partial x^2} - \alpha \beta \quad (1a)$$

$$\frac{\partial \beta}{\partial t} = \frac{\partial^2 \beta}{\partial x^2} + \alpha \beta - k\beta \quad (1b)$$

if we assume quadratic autocatalysis.

For our purposes, we transform the above set into

$$LA + B = AB \quad (2a)$$

$$LB + KB = AB \quad (2b)$$

with $A = 1 - \alpha$, $B = \beta$, $K = 1 - k$ and

$$L = \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial t}.$$

The required boundary conditions are: $A \rightarrow A_s$ ($0 < A_s \leq 1$) for $x \rightarrow -\infty$, $A \rightarrow 0$ for $x \rightarrow +\infty$ and $B \rightarrow 0$ for $|x| > \lambda$. The latter condition expresses the fact that B must represent a localized quantity.

In the absence of linear decay ($k = 0$ or $K = 1$), it is easily observed that the quantity A , as well as B , satisfy the same dynamical equation

$$LF + F = F^2 \quad (3)$$

which is known as Fisher's equation.

A travelling wave solution of this equation reads:

$$F = (1/4) \left\{ 1 - \tanh \left[\frac{1}{2\sqrt{6}} \left(x - \frac{5}{\sqrt{6}} vt \right) \right] \right\}^2 \tag{4}$$

and was obtained by Ablowitz and Zepetella (1979) with a series solution and a non-trivial expansion, by Wang (1988) using an ingenious trick and by Hereman and Takaoko (1990) with an exponential series method.

Notice that $F \rightarrow 1$ for $x \rightarrow -\infty$ and $F \rightarrow 0$ for $x \rightarrow +\infty$. The quantity A in this limit thus retains the required boundary condition as mentioned before. On the other hand, the quantity B loses its localized property if $K = 1$. We will come back to this point later on.

The problem is first tackled with the algebraic method of Hereman *et al* (1990). This systematic method has been used to construct travelling wave solutions of several nonlinear evolution equations. In particular Fisher's equation and related problems are treated successfully.

Hence we start with the following expansions for A and B :

$$A = \sum_{n=1}^{\infty} c_n g^n(\xi) \tag{5a}$$

$$B = \sum_{n=1}^{\infty} d_n g^n(\xi) \tag{5b}$$

with

$$g = \exp(-C\xi) \quad C > 0 \quad \text{and} \quad \xi = x - vt. \tag{6}$$

Upon substitution of these expressions in (2), collecting next all terms with the same power in g , one arrives at an infinite set of nonlinear recursion relations for the coefficients c_n and d_n :

$$(C^2 n^2 - Cnv)c_n + d_n - \sum_{m=1}^{n-1} c_m d_{n-m} = 0 \tag{7a}$$

$$(C^2 n^2 - Cnv)d_n + Kd_n - \sum_{m=1}^{n-1} c_m d_{n-m} = 0. \tag{7b}$$

It is appropriate to choose $c_1 = d_1 = 0$ to get unique values for both C and v . For $n = 2$ and $n = 3$ the nonlinear terms in (7a) and (7b) disappear and (7b) renders the following relations:

$$4C^2 - 2Cv + K = 0. \tag{8}$$

$$9C^2 - 3Cv + K = 0. \tag{9}$$

We remark that the coefficients d_2 and d_3 are now considered as free parameters. From (8) and (9) we get:

$$C = \sqrt{K/6} \quad \text{and} \quad v = 5\sqrt{K/6} \approx 2.04\sqrt{K}. \tag{10}$$

As a consequence, to exhibit travelling waves, only values of K between 0 and 1 are allowed. This fact was also reported by Needham and Merkin (1989).

For $K = 1$ Fisher's case is recovered: $c_i = d_i$ ($i = 2, 3 \dots$); together with the nontrivial choices $d_2 = 1$ and $d_3 = -2$ the series expansion (5a) or (5b) eventually can be written in the following closed form:

$$g(\chi)^2 - 2g(\chi)^3 + 3g(\chi)^4 - \dots = \frac{g(\chi)^2}{(1 + g(\chi))^2} = \frac{1}{4}[1 - \tanh(\chi/2)]^2.$$

with

$$\chi = \lim_{K \rightarrow 1} (C\xi) = (1/\sqrt{6})(x - (5/\sqrt{6})vt). \tag{11}$$

Unfortunately, in the general case that $K \neq 1$, such a summation is not possible because the higher the rank of the coefficients, the more complex the relations become. Moreover we could not find any relevant values for the free parameters. All these facts strongly indicate that in general no closed analytical form for the sought solutions will exist.

In view of the result for $K = 1$, we introduce a series expansion in terms of a tanh function. Such expansions were already used by Huilin and Kelin (1990), to solve a KdV-Burgers type of equation and by Pfersch (1990) to treat a Schrödinger equation.

The solutions we are looking for are supposed to be functions of

$$Y = \tanh(\eta) \quad \text{with} \quad \eta = c(x - vt) \tag{12}$$

whereas the parameter c obviously can be defined as $c = C/2$, in view of the results obtained in Fisher's case (see (10) and (11)). Furthermore, it is convenient to transform also the L operator in terms of this new variable Y :

$$L = (1 - Y^2) \left[(cv - 2c^2Y) \frac{d}{dY} + c^2(1 - Y^2) \frac{d^2}{dY^2} \right]. \tag{13}$$

Now a series expansion in Y can be used conveniently. In a first attempt a straightforward expansion was used. As a result very complicated relations emerge and, in view of the required boundary conditions (for $Y \rightarrow \pm 1$), the results were difficult to interpret.

To handle this problem, we have taken into account the boundary conditions within the series expansion. Therefore the following relations for A and B are introduced:

$$A = (1 - Y)^2 [a_0 + a_1 Y + a_2 Y^2 \dots] \tag{14}$$

$$B = (1 - Y)^2 (1 + Y) [b_0 + b_1 Y + b_2 Y^2 + \dots]. \tag{15}$$

To get Fisher's case, one has to impose also following conditions on the coefficients:

$$a_0 = \frac{1}{4} \quad \text{and} \quad a_i = 0 \quad (i = 1, 2, 3, \dots) \tag{16}$$

$$b_0 = \frac{1}{4} \quad \text{and} \quad b_{2j} = -b_{2j+1} \quad (j = 0, 1, 2) \tag{17}$$

for $K = 1$.

The quantities A and B in this case coincide with the solution F of Fisher's equation (see (4) or (11)).

Upon substitution of (14) and (15) into (2a) and (2b), together with the transformation formula (13), we obtain recursion relations among the coefficients of both expansions.

After some algebra we get from (2a) in lowest order (i.e. the Y^0 term):

$$-\frac{3}{4}Ka_0 + \frac{1}{12}Ka_2 - b_0a_0 + b_0 + \frac{1}{4}Ka_1 = 0. \tag{18}$$

Similarly, from (2b) we get the recursion relations:

$$Kb_2 + 6Kb_0 - 12b_0a_0 + 4Kb_1 = 0 \tag{19}$$

and

$$10Kb_1 - 12b_0a_1 - 12b_1a_0 + 10Kb_2 + 3Kb_3 = 0 \tag{20}$$

by equating the terms in Y^0 and Y^1 respectively. If necessary, the other relations can be found as well.

Due to the number of unknowns and the occurrence of cross terms in these relations, they are obviously difficult to solve. Fortunately, the coefficients we are looking for have to satisfy the above-mentioned conditions (16) and (17) in the limit $K \rightarrow 1$. It will direct us to perform these cumbersome calculations. As a first example, if we restrict the calculations to the relations given above, we have found the following values for the coefficients:

$$a_0 = \frac{K}{4} \quad a_1 = -\left(\frac{K}{4}\right)(1-K) \quad \text{and} \quad a_i = 0 \quad (i \geq 2) \tag{21}$$

$$b_0 = \frac{K^2}{4} \quad b_1 = -\left(\frac{K^2}{4}\right) + \frac{K^2}{22}(1-K) \quad b_2 = \frac{K^2}{4} - \frac{2K^2}{11}(1-K) \tag{22}$$

$$b_3 = -\frac{K^3}{4} \quad b_j = 0 \quad (j \geq 4).$$

Because the number of unknowns exceed the number of relations, other values for the coefficients could be found as well; here we have put forward an approximation valid for small K values. This leads to the approximate solutions:

$$A \approx \left(\frac{K}{4}\right)(1-Y)^2[1-(1-K)Y] \tag{23}$$

$$B \approx \left(\frac{K^2}{4}\right)(1-Y^2)(1-Y)[1 - \left(\frac{9}{11} + \frac{2}{11}K\right)Y + \left(\frac{3}{11} + \frac{8}{11}K\right)Y^2 - KY^3] \tag{24}$$

with $Y = \tanh(K/2\sqrt{6})(x - 5\sqrt{K/6}vt)$.

Obviously, the more one should approach the limit $K \rightarrow 1$, the more coefficients and recursion relations one has to include in the calculations. Further investigations are needed to elaborate this in more detail. Finally, we are able to compare the analytical results (23) and (24) with the numerical calculations of Merkin and Needham (1989), which are particularly detailed in the case that $K = 1/2$:

	<u>Numerical results</u>	<u>Analytical results</u>	
$0 < K \leq 1$:	travelling waves	same	
	velocity: $v = 2\sqrt{K}$	$v = 5\sqrt{K/6} = 2.04\sqrt{K}$	(25)
	$A(Y \rightarrow 1) = 0$	$A(Y \rightarrow 1) = 0$	(26)
$K = \frac{1}{2}$:	$A(Y \rightarrow -1) = A_s = 0.773$	$A(Y \rightarrow -1) = A_s = 0.75$	(27)
	B : asymmetric sech form	same	(28)
	$B_{\max} \approx 1.36$	$B_{\max} \approx 1.21$.	(29)

Moreover, the boundary condition $A(Y \rightarrow -1) = A_s$ applied to (23) agrees fully with the numerical results for $0 < K \leq 1/2$. As a conclusion, we have set up a series expansion for the travelling wave solutions of coupled reaction-diffusion equations. The velocity and the width of these waves are determined. If one closes the hierarchy of relations, preliminary calculations lead to analytical solutions, which for small decay parameters agree well with the numerical computations.

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