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A two-step conditionally bounded numerical integrator to approximate some traveling-wave solutions of a diffusion-reaction equation

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We develop a finite-difference scheme to approximate the bounded solutions of the classical Fisher–Kolmogorov–Petrovsky–Piskunov equation from population dynamics, in which the nonlinear reaction term assumes a generalized logistic form. Historically, the existence of wave-front solutions for this model is a well-known fact; more generally, the existence of solutions of this equation which are bounded between 0 and 1 at all time, is likewise known, whence the need to develop numerical methods that guarantee the positivity and the boundedness of such solutions follows necessarily. The method is implicit, relatively easy to implement, and is capable of preserving the positivity and the boundedness of the new approximations under a simple parameter constraint. The proof of the most important properties of the scheme is carried out with the help of the theory of M-matrices. Finally, the technique is tested against some traveling-wave solutions of the model under investigation; the results evince the fact that the method performs well in the cases considered.

1. Introduction

R. A. Fisher [1937] and A. Kolmogorov, I. Petrovsky and N. Piskunov [Kolmogorov et al. 1937] were the first to investigate the advance wave of mutant genes which are advantageous to some populations distributed on linear habitats. The model that they investigated is known as the Fisher–Kolmogorov–Petrovsky–Piskunov equation, the Fisher–KPP equation, or simply Fisher's equation, and it is one of the simplest diffusive equations with nonlinear reaction. This parabolic partial differential equation is a useful model in the description of the process of epidermal wound healing [Sherratt and Murray 1990], in the theory of the electrodynamics of

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semiconductors [Wallace 1984], in the investigation of excitons [Rashba and Sturge 1982], and as a model for neutron flux in nuclear reactor kinetics [Kastenberg and Chambré 1968].

The Fisher–KPP equation, like many other equations in mathematical physics, is well-known to possess traveling-wave solutions [Wang 1988]. The wave fronts connect the two stationary solutions, 0 and 1 in the equation's nondimensionalized version, via a monotone solution bounded within (0, 1) at all times. The existence of other bounded solutions for this model, apart from traveling waves, is also a standard result in the specialized literature [Wazwaz and Gorguis 2004]. This and the fact that the Fisher–KPP equation is a model for which there is no analytic solution for every admissible set of initial conditions justify interest in the design of numerical techniques preserving the boundedness of the solutions.

The design of numerical methods that preserve several physical or mathematical properties of the phenomena that they describe is a fruitful avenue of research in scientific computation. Thus, from the physical point of view, several methods have been proposed to approximate the solution and the energy dynamics of conservative [Furihata 2001] and dissipative [Furihata 1999] systems. From the mathematical point of view, the preservation of conditions such as symmetry, monotonicity, positivity and boundedness is sometimes a highly desirable characteristic in a numerical integrator. In fact, several numerical methods have been designed with these conditions in mind, particularly in those cases when the variable of interest is measured in an absolute scale. In these situations, the conditions of positivity and boundedness of solutions, which are typical in the study of some traveling waves, arise as constraints in the meaningfulness of the numerical results.

In this article we develop a finite-difference scheme to approximate bounded positive solutions to the Fisher–KPP equation, and test our method against known traveling-wave solutions. The main properties of our technique are consequences of the theory of M-matrices [Fujimoto and Ranade 2004], which are nonsingular, square matrices with the property that their inverses have only positive entries.

This work is organized as follows: In Section 2, we introduce the quantitative model under investigation (namely, the Fisher–KPP equation from population dynamics), and a family of traveling-wave solutions used in the sequel as comparison paradigms. Section 3 presents the numerical method employed to approximate solutions of the problem under investigation. There we prove our main result, which gives parameter conditions under which the method is able to preserve positivity and boundedness of the solutions of the Fisher–KPP model. Section 4 presents numerical evidence that the method is capable of preserving the properties mentioned above when the conditions of our main result are satisfied. We make some concluding remarks in Section 5.

2. The Fisher–KPP equation

Let p be a positive integer. Let $\mathbb{R}^+$ represent the set of nonnegative numbers, and let $I = [a, b]$ be a closed and bounded interval of $\mathbb{R}$. Let u be a real function defined on $I \times \mathbb{R}^+$ which, for practical purposes, is supposed to be twice differentiable in the interior of its domain. In this work, we approximate traveling-wave solutions of the classical Fisher–KPP equation, which, in nondimensional form, is the nonlinear, parabolic partial differential equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + uf(u), \tag{1}$$

where the function $f : \mathbb{R} \to \mathbb{R}$ has the generalized logistic form

$$f(u) = 1 - u^p. \tag{2}$$

As mentioned in the Introduction, this equation was first studied in the context of the dynamics of populations in a one-dimensional, unbounded habitat. (In the original studies, the exponent p was equal to 1.) For every real constant C, the functions

$$u(x,t) = \left\{ \frac{1}{2} \tanh\left[-\frac{p}{2\sqrt{2p+4}} \left(x - \frac{p+4}{\sqrt{2p+4}} t \right) + \frac{C}{2} \right] + \frac{1}{2} \right\}^{2/p} \tag{3}$$

are traveling wave solutions to (1), bounded in the interval $(0, 1)$, and connecting the two constant solutions $u = 0$ and $u = 1$ (see [Wang 1988]). These solutions will be employed for comparison purposes in Section 4.

3. Numerical method

For the discretization, we consider a uniform partition $a = x_0 < x_1 < \cdots < x_N = b$ of the interval I and a uniform partition $0 = t_0 < t_1 < \cdots < t_M = T$ of the time interval $[0, T]$ over which we will compute approximate solutions of (1). We let u_n^k represent the approximation to the exact value of $u(x_n, t_k)$. For convenience, let $\Delta x = (b-a)/N$ and $\Delta t = T/M$, and consider the standard linear operators

$$\delta_t u_n^k = \frac{u_n^{k+1} - u_n^k}{\Delta t}, \tag{4}$$

defined for every $n \in \{0, 1, \ldots, N\}$ and every $k \in \{0, 1, \ldots, M-1\}$, and

$$\delta_x^2 u_n^k = \frac{u_{n+1}^k - 2u_n^k + u_{n-1}^k}{(\Delta x)^2}, \tag{5}$$

defined for every $n \in \{1, 2, \ldots, N-1\}$ and every $k \in \{0, 1, \ldots, M\}$. Let $n \in \{1, 2, \ldots, N-1\}$ and $k \in \{0, 1, \ldots, M-1\}$. With this notation at hand, we

approximate the exact solution of u at (x_n, t_k) through the nonlinear difference equation

$$\delta_t u_n^k = \delta_x^2 u_n^{k+1} + u_n^{k+1} f(u_n^k). \tag{6}$$

Clearly, in order to approximate solutions of (1) using the numerical method (6), appropriate initial and boundary conditions must be imposed in both the continuous and the discrete scenarios. In the present work, we will consider an initial profile of the form $u(x, 0) = \phi(x)$ for every $x \in I$, a condition that translates to the discrete scene into the constraint $u_n^0 = \phi(x_n)$, for $n \in \{0, 1, \ldots, N\}$. Similarly, we will consider boundary conditions of the form $u(a, t) = g(t)$ and $u(b, t) = h(t)$ for every $t \in [0, T]$, which translate, respectively, as $u_0^k = g(t_k)$ and $u_N^k = h(t_k)$, for every $k \in \{0, 1, \ldots, M\}$. With these conventions, the finite-difference method (6) may be rewritten in vector form as the equation

$$A_k \boldsymbol{u}^{k+1} = \boldsymbol{v}^k \quad \text{for } k \in \{0, 1, \ldots, M-1\}, \tag{7}$$

where $\boldsymbol{v}^k$ is the $(N+1)$-dimensional real vector

$$\boldsymbol{v}^k = \left(g(t_{k+1}), u_1^k, \ldots, u_{N-1}^k, h(t_{k+1})\right)^t, \tag{8}$$

for $k \in \{0, 1, \ldots, M\}$, and A is the matrix of size $(N+1) \times (N+1)$ given by

$$A_k = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ -R & a_1^k & -R & 0 & \cdots & 0 & 0 & 0 \\ 0 & -R & a_2^k & -R & \cdots & 0 & 0 & 0 \\ 0 & 0 & -R & a_3^k & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & a_{N-2}^k & -R & 0 \\ 0 & 0 & 0 & 0 & \cdots & -R & a_{N-1}^k & -R \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{pmatrix}. \tag{9}$$

Here,

$$R = \frac{\Delta t}{(\Delta x)^2}, \tag{10}$$

$$a_n^k = 1 + 2R - f(u_n^k)\Delta t \quad \text{for } n \in \{1, 2, \ldots, N-1\}. \tag{11}$$

The forward-difference stencil of our method is depicted in Figure 1. The method is clearly implicit and, after appropriate boundary conditions are specified at the endpoints of I, it only requires of an initial profile $\boldsymbol{u}^0$ in order to compute the subsequent approximations. Note also that, if f were a constant function, the matrix A_k would be a constant matrix A, and the approximation at time k would be given by $A^k \boldsymbol{u}^k = \boldsymbol{u}^0$.

We now establish conditions under which the finite-difference method (6) pre-

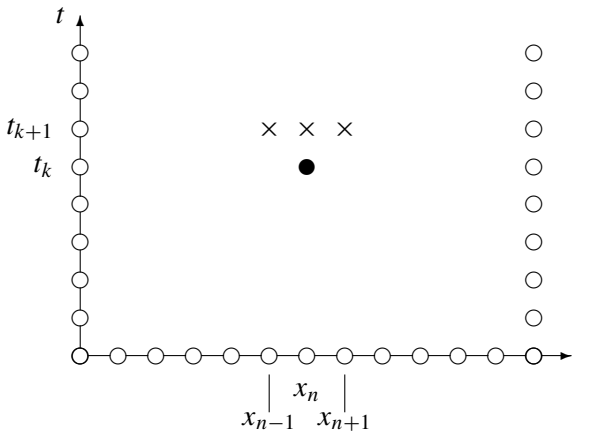

Figure 1. Forward-difference stencil of the finite-difference scheme (6). The black circle represents the known approximation to the exact solutions at the time t_k, and the crosses denote the unknown, new approximations at the time t_{k+1}.

serves the boundedness and the positivity of the solutions of (1), and it makes use of the nonsingularity properties of M-matrices [Fujimoto and Ranade 2004].

Proposition 1. *Let $k \in \{0, 1, \ldots, M-1\}$, let p be equal to 1, and suppose that all the components of $\boldsymbol{v}^k$ are numbers in $(0, 1)$. If $\Delta t < 1$ then the components of $\boldsymbol{u}^{k+1}$ in (7) are all likewise bounded in $(0, 1)$.*

Proof. Clearly, A_k has nonpositive, off-diagonal entries. Moreover, if $f(u_n^k)\Delta t < 1$ for every $n \in \{1, 2, \ldots, N-1\}$, then A_k is a strictly diagonally dominant matrix with positive diagonal entries (notice that such condition holds if $0 < u_n^k < 1$ for every $n \in \{1, 2, \ldots, N-1\}$ and $\Delta t < 1$) and, as a consequence, A_k is an M-matrix, that is, a nonsingular matrix whose inverse only has positive entries. Together with (7), this implies that $\boldsymbol{u}^{k+1}$ is a vector with positive entries. Next, we establish the boundedness from above of the components of $\boldsymbol{u}^{k+1}$. Let $\boldsymbol{e}$ be the $(N+1)$-dimensional vector all of whose components are equal to 1, and let $\boldsymbol{w}^{k+1} = \boldsymbol{e} - \boldsymbol{u}^{k+1}$. A simple substitution in (7) gives us the equation

$$A_k \boldsymbol{w}^{k+1} = A_k \boldsymbol{e} - \boldsymbol{v}^k. \tag{12}$$

The first and last components of the right-hand side of (12) are, respectively, $1-g(t_k)$ and $1-h(t_k)$, which are positive, while for every $n \in \{1, 2, \ldots, N-1\}$, the $(n+1)$-st component is given by the expression $(1-\Delta t)(1-u_n^k)$, which is also a positive number. As in the first part of this proof, it follows that the components of $\boldsymbol{w}^{k+1}$ are all positive numbers or, equivalently, that the components of $\boldsymbol{u}^{k+1}$ are all less than 1. □

We stress that (4) is a first-order accurate approximation of the partial derivative of u with respect to t at (x_n, t_k), and that (5) is an approximation of the second order to the value of the partial derivative of u with respect to x^2 at the same point. Under these circumstances, the linearized version of the finite-difference scheme (6) is consistent of order $\Delta t + (\Delta x)^2$ with the linearized version of (1) at (x_n, t_{k+1}).

4. Numerical results

To illustrate the validity of the our method and its computational implementation, we ran two numerical experiments, choosing the initial conditions so the exact solution is known, namely, the function (3). We set $C = 1$ and $p = 1$, and let the spatial domain be $I = [-50, 150]$, imposing at the endpoints Dirichlet conditions provided by the exact solution evaluated at -50 and 150.

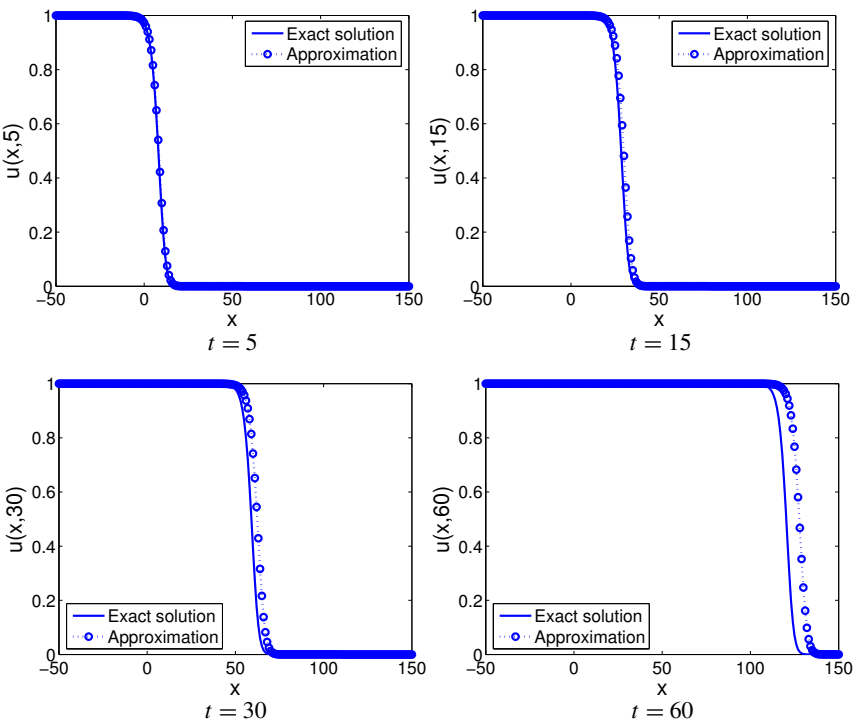

Figure 2. Analytical solution (solid line) and the corresponding approximation (dotted line) versus the spatial variable x at four different times, of a system governed by (1) with $p = 1$. The initial profile is that given by (3) at $t = 0$ with $C = 1$, and the boundary conditions are provided by (3) at the endpoints of $[-50, 150]$ at any time. Numerically, the method (6) employed $\Delta x = 1$ and $\Delta t = 0.05$, and the times considered were $t = 5, 15, 30, 60$.

In the first run, we use the finite-difference method (6) with $\Delta x = 1$ and $\Delta t = 0.05$, so that the parameter constraint in Proposition 1 for the boundedness of the method be satisfied. Under these conditions, Figure 2 compares the exact solutions with the corresponding numerical approximations provided by our technique at four different times, namely $t = 5$, 15, 30 and 60. The results show that the computational solution remains bounded within (0, 1), as expected. Additionally, there exists a good agreement between both solutions at small times; the difference between the exact solutions and the numerical approximations is more pronounced at the times $t = 30$ and 60.

In the second run, we change only the parameter values $\Delta x = 0.5$ and $\Delta t = 0.005$. The numerical results are presented in Figure 3, and one immediately notices a better agreement between the analytical solutions and the computational approximations

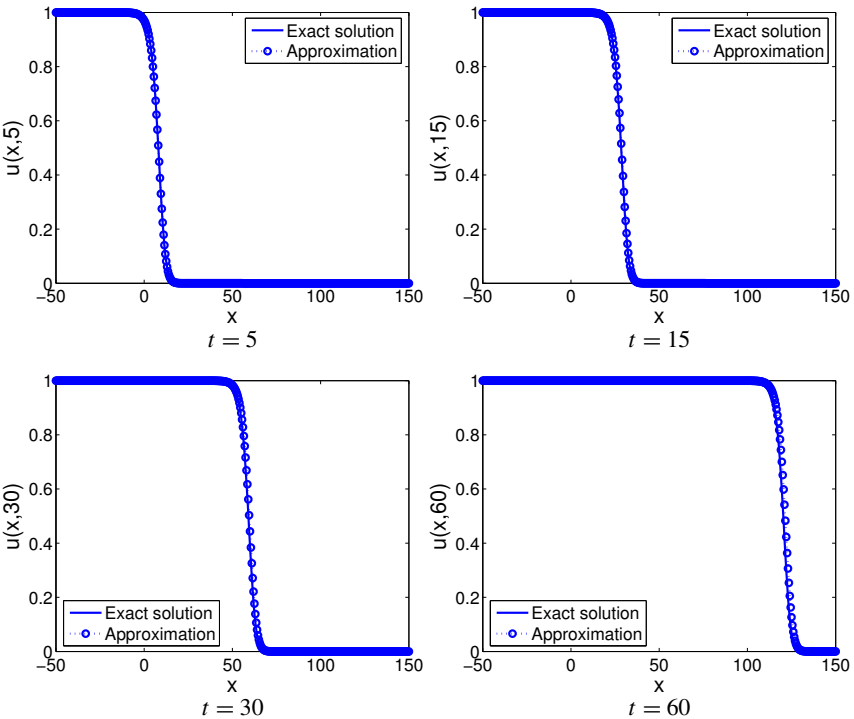

Figure 3. Analytical solution (solid line) and the corresponding approximation (dotted line) versus the spatial variable x at four different times, of a system governed by (1) with $p = 1$. The initial profile is that given by (3) at $t = 0$ with $C = 1$, and the boundary conditions are provided by (3) at the endpoints of $[-50, 150]$ at any time. Numerically, the method (6) employed $\Delta x = 0.5$ and $\Delta t = 0.005$, and the times considered were $t = 5$, 15, 30, 60.

to the problem under consideration, even for larger values of time. We also see that the numerical approximations, like the exact solutions, remain bounded within $(0, 1)$. This is in agreement with Proposition 1.

5. Conclusions

We have presented a numerical method to approximate bounded solutions of the classical Fisher–KPP equation from population dynamics. The proposed finite-difference scheme is a nonstandard method in the way that the reaction term is approximated, and it may be conveniently expressed in vector form in terms of the multiplication by a tridiagonal matrix which, under certain circumstances, is actually an M-matrix. In this way, new approximations may be written as the product of the previous approximation by the inverse of the M-matrix. Some simple and direct calculations show that the new approximations are bounded between 0 and 1 under suitable conditions on the computational parameters.

The method was implemented and tested against known exact solutions of the classical Fisher–KPP equation on a bounded spatial domain. The results show that the method performs well when approximating the analytical solutions considered. Moreover, one notices that the method preserves the boundedness and the positivity of the solutions considered when the parameter conditions derived in the work are satisfied.

References

[Fisher 1937] R. A. Fisher, "The wave of advance of advantageous genes", *Ann. Eugenics* **7** (1937), 355–369.

[Fujimoto and Ranade 2004] T. Fujimoto and R. R. Ranade, "Two characterizations of inverse-positive matrices: the Hawkins–Simon condition and the Le Chatelier–Braun principle", *Electron. J. Linear Algebra* **11** (2004), 59–65. MR 2005m:15053 Zbl 1069.15020

[Furihata 1999] D. Furihata, "Finite difference schemes for $\partial u/\partial t = (\partial/\partial x)^{\alpha}\delta G/\delta u$ that inherit energy conservation or dissipation property", *J. Comput. Phys.* **156**:1 (1999), 181–205. MR 2000j:65076 Zbl 0945.65103

[Furihata 2001] D. Furihata, "Finite-difference schemes for nonlinear wave equation that inherit energy conservation property", *J. Comput. Appl. Math.* **134**:1-2 (2001), 37–57. MR 2002g:65096 Zbl 0989.65099

[Kastenberg and Chambré 1968] W. E. Kastenberg and P. L. Chambré, "On the stability of nonlinear space-dependent reactor kinetics", *Nucl. Sci. Eng.* **31** (1968), 67–79.

[Kolmogorov et al. 1937] A. Kolmogoroff, I. Petrovsky, and N. Piscounoff, "Étude de l'équation de la diffusion avec croissance de la quantité de matière et son application a un problème biologique", *Bull. Univ. Moscou, Ser. Internat. A* **1**:6 (1937), 1–25. Zbl 0018.32106

[Rashba and Sturge 1982] E. I. Rashba and M. D. Sturge (editors), *Excitons*, North-Holland, Amsterdam, 1982.

[Sherratt and Murray 1990] J. A. Sherratt and J. D. Murray, "Models of epidermal wound healing", *Proc. R. Soc. Lond. B* **241** (1990), 29–36.

[Wallace 1984] P. R. Wallace, *Mathematical analysis of physical problems*, Dover Publications, New York, 1984. MR 86c:00006 Zbl 1092.00501

[Wang 1988] X. Y. Wang, "Exact and explicit solitary wave solutions for the generalised Fisher equation", *Phys. Lett. A* **131**:4-5 (1988), 277–279. MR 89h:35320

[Wazwaz and Gorguis 2004] A.-M. Wazwaz and A. Gorguis, "An analytic study of Fisher's equation by using Adomian decomposition method", *Appl. Math. Comput.* **154**:3 (2004), 609–620. MR 2005c:35152 Zbl 1054.65107

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