Computing the Drift of Mutant Genes

Olmos-Gomez, Miguel A
Department of Mathematics
Universidad de Guadalajara
Mexico
miguel.olmos@cucei.udg.mx

Arriaga-Gutierrez, Ma Merced
Department of Mathematics
Universidad de Guadalajara
Mexico
mercedarriaga@hotmail.com

Manoranjan, Valipuram S.
Department of Mathematics
Washington State University
Pullman, WA 99164-3113
mano@wsu.edu

Abstract - We develop a numerical scheme for computing the solution of a generalized version of Fisher's equation. The main idea is to use a modified Crank-Nicolson method in order to construct a predictor corrector scheme. Then incorporate variable boundary conditions that mimic the asymptotic behavior of the initial condition in order to ensure that the wave has the right speed as it advances.

Keywords: Fisher's equation, traveling waves, analytical solutions, finite-difference, numerical solution

1 Introduction

Nonlinear reaction-diffusion equations play fundamental roles in a great variety of situations such as heat/mass transfer, developmental biology, chemical reactions, and genetic processes. In this paper we consider a particular reaction-diffusion equation known as the generalized Fisher's equation. This equation describes the drift of advantageous genes due to favorable local conditions for mutation. It is seen that the asymptotic conditions at the extreme back of the advancing drift wave (where the numbers of the mutant genes are small) can determine the speed of advance.

The generalized Fisher's problem we consider is

$$u_t = u_{xx} + u - u^p, p > 1 \tag{1}$$

$$\lim_{x \to -\infty} u(x,t) = 0, \lim_{x \to \infty} u(x,t) = 1, t > 0, u(x,0) = u_0(x) \tag{2}$$

Following Larson [9], if the initial condition $u_0(x) \in [0,1], x \in \mathbb{R}$ and $u_0(x) \backsim \lambda e^{\beta x}, \lambda > 0$ as $x \to -\infty$, it can been shown that for every $\beta \in (0,1)$ there exists a traveling wave solution to (1) - (2) with speed $c_\beta = \beta + \frac{1}{\beta}$; if $\beta > 1$, the traveling wave solution will have an asymptotic speed of 2; that is, if $u_0(x)$ is a positive function that satisfies the boundary conditions (2) on $\mathbb{R}$ and if

$$u_0(x) \backsim \lambda e^{\beta x}, \lambda > 0 \text{ as } x \to -\infty \tag{3}$$

then as $t \to \infty$, the solution will evolve to a traveling wave with speed $c(\beta)$ where

$$c(\beta) = \begin{cases} \beta + \frac{1}{\beta}, & 0 < \beta \leq 1 \\ 2 & \beta > 1 \end{cases}$$

Also Kolmogorov et al. [7] have shown that if the initial data is chosen such that

$$u_0(x) = \begin{cases} 0, & x < 0, \\ 1, & x > 0, \end{cases}$$

then the solution will approach a traveling wave of speed 2.

We develop a numerical scheme for computing the solution of the generalized Fisher's equation. We construct the boundary conditions so that the asymptotic behavior at the extreme back of the wave is modeled correctly to ensure that the wave advances with the right speed.

It should be noted that the generalized Fisher's equation can also be used to study certain chemical/electrical systems and population growth of various species.

2 Analytical Solutions

This section presents some analytical results for particular values of p in equation (1). In 1979, Ablowitz and Zeppetella [1] found the first known explicit traveling wave solution by substituting $u = u(z) = u(x - ct)$ to obtain the ordinary differential equation

$$u'' + cu' + u(1-u) = 0$$

(when $p = 2$) and solving it. The solution method uses the idea in the classical theory of ordinary differential equations. The solution is of Painlevé type. It is a one parametric family of solutions given by

$$u(x,t) = \frac{1}{\left[1 + c_1 e^{-\frac{1}{\sqrt{6}}\left(x + \frac{5}{\sqrt{6}}t\right)}\right]^2} \tag{4}$$

where c_1 is a parameter and the speed of the wave is $\frac{5}{\sqrt{6}}$. It can be seen that the solution will be unbounded if c_1 is negative. This solution is the only known explicit traveling wave solution for Fisher's equation [1, 5, 8, 11] and corresponds to the asymptotic behavior with $\beta = \frac{2}{\sqrt{6}}$.

Equation (1) is known as the Newell-Whitehead equation when $p = 3$ [2, 3, 4, 10, 11]. The known explicit solutions of Newell-Whitehead equation are given by [11]

$$u(x,t) = \frac{c_1 \exp(\frac{1}{2}\sqrt{2}x) - c_2 \exp\left(-\frac{1}{2}\sqrt{2}x\right)}{c_1 \exp\left(\frac{1}{2}\sqrt{2}x\right) + c_2 \exp\left(-\frac{1}{2}\sqrt{2}x\right) + c_3 \exp\left(-\frac{3}{2}t\right)}, \tag{5}$$

where c_1, c_2, and c_3 are arbitrary constants.

Note that if $c_3 = 0$ in (5), then we have a wave profile with speed $c = 0$, i. e., a steady state solution or a standing wave.

For $p > 1$, if we define $\lambda = \frac{(1-p)(p+3)}{2(p+1)}$ and, $\mu = \frac{(1-p)}{\sqrt{2(p+1)}}$, then the traveling-wave solutions are given by [11]

$$\begin{aligned} u(x,t) &= \left[1 + c_1 \exp(\lambda t \pm \mu x)\right]^{\frac{2}{1-p}} \\ u(x,t) &= \left[-1 + c_1 \exp(\lambda t \pm \mu x)\right]^{\frac{2}{1-p}} \end{aligned}$$

with speed $c = \lambda/\mu = \frac{p+3}{\sqrt{2p+2}}$.

It can be seen that for the case $p = 2$ we have $\lambda = -\frac{5}{6}$ and $\mu = -\frac{1}{\sqrt{6}}$ which agrees with the solution given in [1]. If $p = 3$, we have $\lambda = -\frac{3}{2}$ and $\mu = -\frac{1}{\sqrt{2}}$ which is consistent with (5) when $c_2 = 0$ or $c_1 = 0$.

3 Numerical Scheme

Let us consider the equation

$$u_t = \phi(x, t, u, u_x, u_{xx}), x \in \mathbb{R}, 0 < t \le T \tag{6}$$

subject to smooth initial and boundary conditions.

The Crank-Nicolson scheme for equation (6) is given by

$$\begin{aligned} u_m^{n+1} &= u_m^n \\ &+ k\phi\left(mh, nk, \frac{u_m^{n+1} + u_m^n}{2}, \frac{\frac{u_{m+1}^{n+1}+u_{m+1}^n}{2} - \frac{u_{m-1}^{n+1}+u_{m-1}^n}{2}}{2h}, \frac{\frac{u_{m+1}^{n+1}+u_{m+1}^n}{2} - 2\frac{u_m^{n+1}+u_m^n}{2} + \frac{u_{m-1}^{n+1}+u_{m-1}^n}{2}}{h^2}\right), \end{aligned} \tag{7}$$

while an explicit scheme is

$$u_m^{n+1} = u_m^n + k\phi\left(mh, nk, u_m^n, \frac{u_{m+1}^n - u_{m-1}^n}{2h}, \frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{h^2}\right). \tag{8}$$

For the generalized Fisher's equation (7) reduces to

$$
\begin{aligned}
u_m^{n+1} &= u_m^n + \frac{k}{h^2}\left(\frac{u_{m+1}^{n+1}+u_{m+1}^n}{2} - 2\frac{u_m^{n+1}+u_m^n}{2} + \frac{u_{m-1}^{n+1}+u_{m-1}^n}{2}\right) \\
&\quad + k\left(\frac{u_m^{n+1}+u_m^n}{2}\right) - k\left(\frac{u_m^{n+1}+u_m^n}{2}\right)^p .
\end{aligned} \tag{9}
$$

This scheme is implicit and we need to solve a nonlinear system of equations at every time step. To avoid solving nonlinear systems several times we construct a predictor-corrector scheme.

This predictor-corrector scheme is

$$
\begin{aligned}
w_m^{n+1} &= u_m^n + \frac{k}{h^2}\left(\frac{w_{m+1}^{n+1}+u_{m+1}^n}{2} - 2\frac{w_m^{n+1}+u_m^n}{2} + \frac{w_{m-1}^{n+1}+u_{m-1}^n}{2}\right) \\
&\quad + k u_m^n - k\left(u_m^n\right)^p . \\
u_m^{n+1} &= u_m^n + \frac{k}{h^2}\left(\frac{u_{m+1}^{n+1}+u_{m+1}^n}{2} - 2\frac{u_m^{n+1}+u_m^n}{2} + \frac{u_{m-1}^{n+1}+u_{m-1}^n}{2}\right) \\
&\quad + k\left(\frac{w_m^{n+1}+u_m^n}{2}\right) - k\left(\frac{w_m^{n+1}+u_m^n}{2}\right)^p .
\end{aligned}
$$

For convenience, let us rewrite the scheme as

$$
\begin{aligned}
-\frac{r}{2}w_{m-1}^{n+1} + (1+r)\,w_m^{n+1} - \frac{r}{2}w_{m+1}^{n+1} &= \frac{r}{2}u_{m-1}^n + (1-r)\,u_m^n + \frac{r}{2}u_{m+1}^n \\
&\quad + k u_m^n - k\left(u_m^n\right)^p .
\end{aligned} \tag{P}
$$

$$
\begin{aligned}
-\frac{r}{2}u_{m-1}^{n+1} + (1+r)\,u_m^{n+1} - \frac{r}{2}u_{m+1}^{n+1} &= \frac{r}{2}u_{m-1}^n + (1-r)\,u_m^n + \frac{r}{2}u_{m+1}^n \\
&\quad + k\left(\frac{w_m^{n+1}+u_m^n}{2}\right) - k\left(\frac{w_m^{n+1}+u_m^n}{2}\right)^p .
\end{aligned} \tag{C}
$$

where $r = \frac{k}{h^2}$.

Typically, this numerical scheme will have better stability properties and at least the same order of consistency as the explicit finite-difference (8).

The numerical computations were carried out over the finite domain $[-L, L]$ for large L. We impose boundary conditions that mimic the asymptotic behavior consistent with the initial data. The boundary conditions used are

$$
u(-L,t) = \frac{1}{2}e^{\beta(-L-c_n t)}, u(L,t) = 1 \tag{10}
$$

where c_n is the computed speed of the left front at time $t = t_n$. The speed of the wave is computed by monitoring the point $(x_c, u(x, t_n)) = \left(x_c, \frac{1}{2}\right)$. We used cubic interpolation in order to get the point where the numerical solution is equal to $\frac{1}{2}$.

If the initial value is

$$
u_0(x) = \begin{cases} 0, & x < 0, \\ 1, & x > 0, \end{cases}
$$

the predicted speed is $c = 2$ and we will use $u(-L,t) = 0$ in (10).

When the initial value is given by the exact solution to (1):

$$
u(x,t) = \left[1 + c_1 \exp(\lambda t \pm \mu x)\right]^{\frac{2}{1-p}}
$$

the speed c is $\frac{\lambda}{\mu} = \frac{p+3}{\sqrt{2p+2}}$ and the corresponding β is $\sqrt{\frac{2}{p+1}}$.

The mesh width h and the time step k are chosen according to the stability criteria given by

$$
h \le 1, k \le \frac{h^2}{4+2h^2}.
$$

These criteria were derived by requiring the numerical scheme (8) to preserve monotonicity of the solution profile.

4 Numerical Results

We applied the predictor-corrector scheme with the initial condition

$$u_0(x) = \begin{cases} \frac{1}{2}e^{\beta x}, & x < 0, \\ 1 - \frac{1}{2}e^{-\beta x}, & x > 0, \end{cases}$$

for any $p > 1$. The speed of the computed front should be $c(\beta) = \beta + \frac{1}{\beta}$. The mesh width and the time step size where chosen as $h = 1$ and $k = 0.1$ satisfying the stability criteria.

For $\beta = 0.2$ we have that the predicted speed c is 5.2, therefore the front will reach the boundary at $t \approx \frac{200}{5.2} = 38.46$. We applied the predictor-corrector method for $t \in [0, 36]$. The graphs of the solutions and the computed speeds for several p-values are given below.

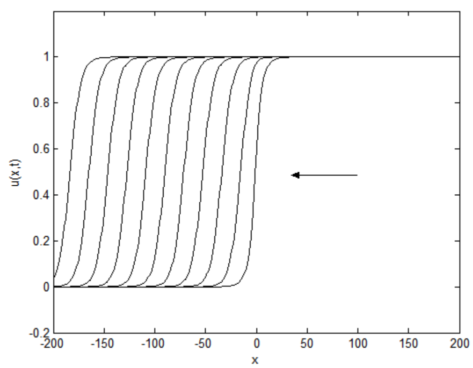


Figure 1: Approximated solution at $t = 36, p = 2$

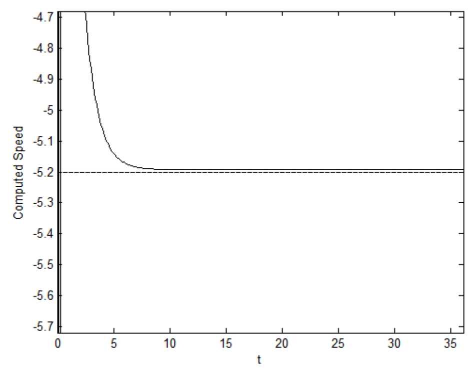


Figure 2: Exact speed $= -5.2$

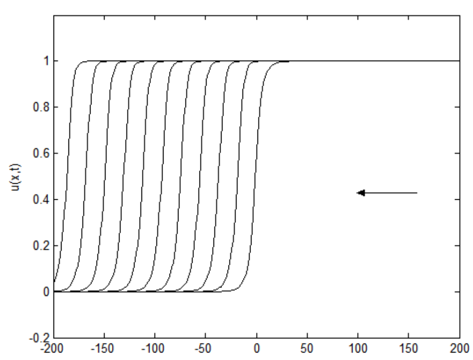


Figure 3: Approximated solution at $t = 36, p = \pi$

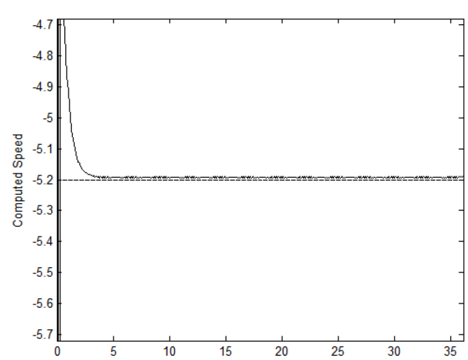


Figure 4: Exact speed $= -5.2$

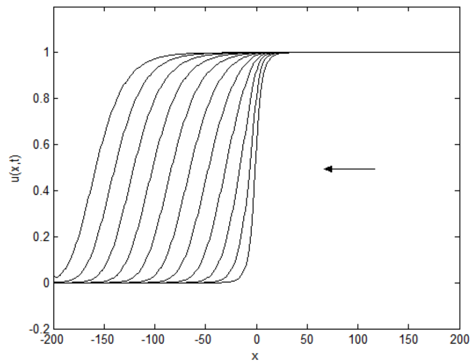


Figure 5: Approximated solution at $t = 36, p = 1.3$

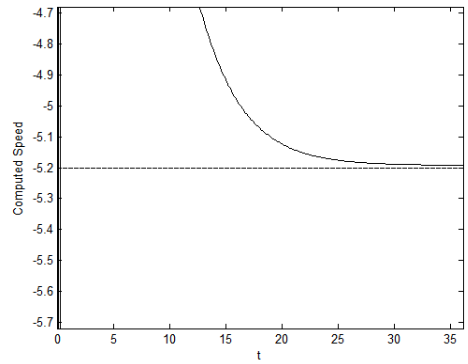


Figure 6: Exact speed $= -5.2$

When $\beta > 1$, for different p values, we obtained a computed speed close to 2 as the theoretical results state. If we apply the initial condition

$$u_0(x) = \begin{cases} 0, & x < 0, \\ 1, & x > 0, \end{cases}$$

the predicted speed is 2 and the time it takes for the front to reach the boundary is $t = 100$. We computed the solution for $t \in [0, 80]$. We also changed the value of h to $h = 0.05$ in order to get a better approximation to the predicted speed.

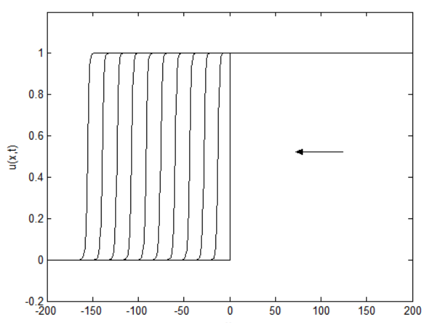


Figure 7: Approximated solution at $t = 80, p = 5$

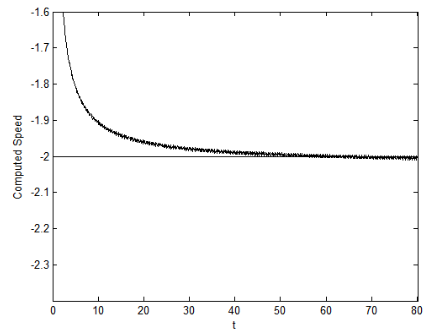


Figure 8: Exact speed $= -2$

We also used as initial condition

$$u_0(x) = \begin{cases} \frac{1}{2}e^{\beta x}, & x < 0, \\ \frac{1}{2}e^{-\gamma x}, & x > 0, \end{cases}$$

where β and γ are positive numbers. This condition will generate two profiles, one traveling to the left with speed $\beta + \frac{1}{\beta}$, and the second one traveling to the right with speed $\gamma + \frac{1}{\gamma}$. A typical computed solution is given in the figures below. The values for β and γ in the figures are 0.4 and 0.2 respectively.

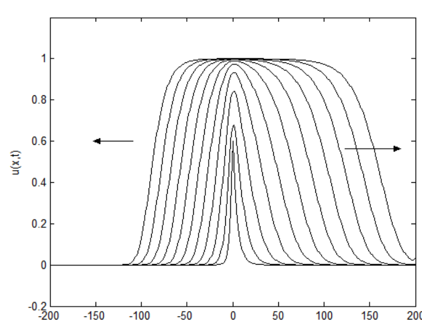
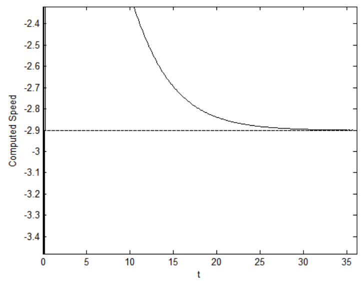


Figure 9: Approximated solution at $t = 36, p = 1.3$



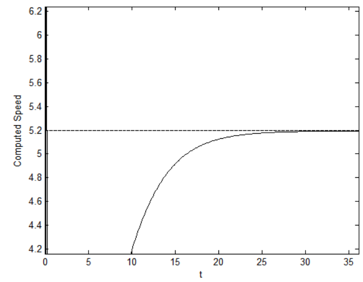


Figure 10: Exact speed of the left front $= -2.9$ Figure 11: Exact speed of the right front $= 5.2$

As noted in section 2, when $p = 3$, the exact solution solution (as time increases)

$$u(x,t) = \frac{c_1 \exp(\frac{1}{2}\sqrt{2}x) - c_2 \exp\left(-\frac{1}{2}\sqrt{2}x\right)}{c_1 \exp\left(\frac{1}{2}\sqrt{2}x\right) + c_2 \exp\left(-\frac{1}{2}\sqrt{2}x\right) + c_3 \exp\left(-\frac{3}{2}t\right)}$$

becomes a standing wave given by

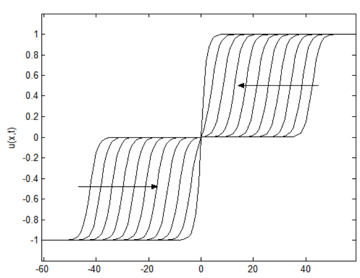
$$u(x,t) = \frac{c_1 \exp(\frac{1}{2}\sqrt{2}x) - c_2 \exp\left(-\frac{1}{2}\sqrt{2}x\right)}{c_1 \exp\left(\frac{1}{2}\sqrt{2}x\right) + c_2 \exp\left(-\frac{1}{2}\sqrt{2}x\right)}$$

The common speed of the fronts is $c = \frac{3}{\sqrt{2}}$ before they reach the form of a standing wave. If we choose $c_1 = c_2 = 1$, this solution is a front from -1 to 1. For p odd, we will use

$$u_0(x) = \frac{\exp(\frac{1}{2}\sqrt{2}x) - \exp\left(-\frac{1}{2}\sqrt{2}x\right)}{\exp\left(\frac{1}{2}\sqrt{2}x\right) + \exp\left(-\frac{1}{2}\sqrt{2}x\right) + \exp(30)}$$

as the initial value.

For $p = 3$ the computed solution is given in the following graphs



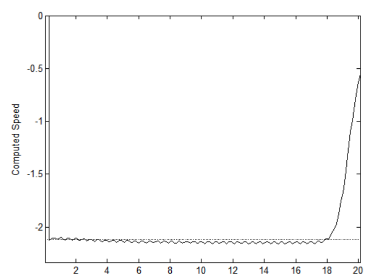
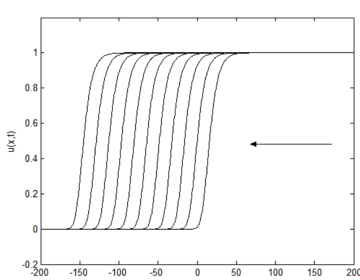


Figure 12: Approximated solution at $t = 20$ Figure 13: Exact speed $= -2.1213$

If the exact solution

$$u(x,t) = \left[1 + c_1 \exp(\lambda t \pm \mu x)\right]^{\frac{2}{1-p}}, c_1 > 0, p > 1$$

is used as the initial condition, we see that the fronts will travel with speed $c = \frac{\lambda}{\mu} = \frac{p+3}{\sqrt{2p+2}}$. The corresponding β value is $\frac{2}{\sqrt{2(p+1)}}$. We have the following numerical results ($h = 0.05$).



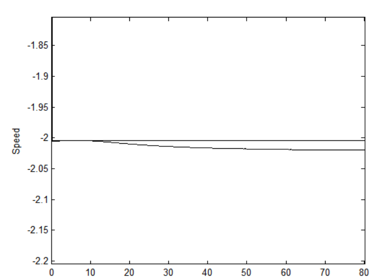


Figure 14: Approximated solution at $t = 80, p = 1.3$ Figure 15: Exact speed $= -2.0049$

5 Conclusions

The predictor-corrector method that we developed seems to have good stability properties and gives more accurate speeds for the traveling fronts. It is better to use cubic interpolation to compute the speed in order to avoid unwanted oscillations.

The use of non-constant boundary conditions that mimic the asymptotic behavior of the initial condition, as we did, allows us to get the traveling fronts closer to the finite boundaries and it is easier to implement than the method given by Hagstrom et al [6]. Also, we do not use the exact speed in the implementation of the boundary conditions- but, the transient speed as the front advances.

From the numerical work carried out we can say that our predictor-corrector method with cubic interpolation and variable boundary conditions is a robust method for the generalized Fisher's equation that gives good approximations to the fronts and their speeds.

6 References

[1] ABLOWITZ, M.J., ZEPPETELLA, A., *Explicit Solutions of Fisher's Equation for a Special Wave Speed*, Bull. Math. Biol., Vol **45**, pp. 835-840, 1979.

[2] CARIELLO, F., TABOR, M., *Painlevé Expansions for Nonintegrable Evolution Equations*, Physica D, Vol. **39**, No. 1, pp. 77–94, 1989.

[3] CICOGNA, G., *"Weak" Symmetries and Adopted Variables for Differential Equations*, Int. J. Geometric Meth. Modern Phys., Vol. **1**, No 1–2, pp. 23–31, 2004.

[4] CLARKSON, P.A., MANSFIELD, E.L., *Symmetry Reductions and Exact Solutions of a Class of Nonlinear Heat Equations*, Physica D, Vol. **70**, No. 3, pp. 250–288, 1994.

[5] DANILOV, V.G., MAZLOV, V.P., VOLOZOV, K.A., *Mathematical Modelling of Heat and Mass transfer Processes*, Kluwer, Dordrecht, 1995.

[6] HAGSTROM, T., KELLER H.B., *The Numerical Calculation of Traveling Wave Solutions of Nonlinear Parabolic Equations*, SIAM J. Sci. Stat. Comput., Vol **7**, No 3, pp. 978-988, 1986.

[7] KOLMOGOROV, A.N., PETROVSKII, I.G., PISKUNOV, N. S., *A Study of the Equation of Diffusion with Increase in the Quantity of Matter and its Application to Biological Problem*, Bull. Univ. Moscow Univ, Ser. Inter., Sec. A, **1**, pp. 1-26, 1937.

[8] KUDRYASHOV, N.A., *On Exact Solutions of Families of Fisher Equations*, Theor. & Math. Phys., Vol. **94**, No. 2, pp. 211-218, 1993.

[9] LARSON, D.A., *Transient Bounds and Time Asymptotic Behavior of Solutions to Nonlinear Equations of Fisher Type*, SIAM J. Appl. Math., Vol **34**, No. 1, pp. 93-103, 1978.

[10] NUCCI, M.C., CLARKSON, P.A., *The Nonclassical Method is More General than the Direct Method for Symmetry Reductions. An Example of the Fitzhugh–Nagumo Equation*, Phys. Lett. A, Vol. **164**, pp. 49–56, 1992.

[11] POLYANIN, A.D., ZAITSEV, V.F. *Handbook of nonlinear Partial Differential Equations*, Chapman & Hall/CRC, Boca Raton, 2004.