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DIRECT AND INDIRECT APPROXIMATIONS TO POSITIVE SOLUTION FOR A NONLINEAR REACTION-DIFFUSION PROBLEM I. DIRECT (VARIATIONAL)

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Abstract. We consider a nonlinear, second-order, two-point boundary value problem that models some reaction-diffusion precesses. When the reaction term has a particular form, $f(u) = u^3$, the problem has a unique positive solution that satisfies a conserved integral condition. We study the bifurcation of this solution with respect to the length of the interval and it turns out that solution bifurcates from infinity. In the first part, we obtain the numerical approximation to the positive solution by *direct* (*variational*) methods, while in the second part we consider *indirect* numerical methods. In order to obtain *directly* accurate numerical approximations to this positive solution, we characterize it by a variational problem involving a conditional extremum. Then we carry out some numerical experiments by usual finite elements method.

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1. INTRODUCTION

We are concerned with the existence, uniqueness and numerical approximations of positive solutions for the semilinear parabolic problem

$$\begin{aligned} &u_t = u_{xx} + u^p, && 0 < x < L, t > 0, \\ &u(0,t) = u(L,t) = 0, && t > 0, \\ &u(x,0) = u_0(x), && 0 < x < L, \end{aligned} \tag{1}$$

where $u_0(x)$ satisfies the compatibility condition $u_0(0) = u_0(L) = 0$, with any real p, $p > 1$ and $L < \infty$. We further assume that (1) has a stationary positive solution $\bar{u}$, i.e. $\bar{u}$ is a solution of boundary value problem

$$\begin{aligned} &u_{xx} + u^p = 0, && 0 < x < L, \\ &u(0) = u(L) = 0. \end{aligned} \tag{2}$$

The stationary problem (2) is in fact the problem 97-8 by Ph. Korman [10]. He invokes a phase-plane analysis to observe that the positive solution $\bar{u}(x)$

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is unique ($\bar{u}(x) > 0$ for $x \in (0, L)$) and asks to show that for $p = 3$ and for any L this solution satisfies

$$\int_0^L \bar{u}(x)\,\mathrm{d}x = \frac{\pi}{\sqrt{2}} \tag{3}$$

which means that the integral of $\bar{u}$ is conserved independently on L.

We have proved in [6] that the solution $\bar{u}(x)$ of (2) satisfies

$$\int_0^L u(x)\,\mathrm{d}x = \sqrt{2(p+1)}\,u_{\max}^{\frac{3-p}{2}}\left(F(1) - F(0)\right), \tag{4}$$

where $F(v)$ is the primitive function of $v/\sqrt{1 - v^{p+1}}$, $v = u/u_{\max}$ and $u_{\max}$ is the maximum value of u on $[0, L]$.

The condition (3) will play a key role in our analysis. This independence of the length of the domain condition can be used successfully to approximate, by a direct or indirect method, the solutions of the problems (1) and (2).

The interest in such stationary solutions, sometimes called dissipative structures, has been occasioned by their possible role in reflecting the corresponding phenomena of pattern formation in developing organisms and in ecological communities. Problems of type (1), in one or more spatial dimensions, have been used also to model some biological phenomenon or technological processes, but we do not go into much detail about applications in the various fields mentioned above (see for example [8]).

The first goal of the present paper is an analysis of bifurcation issue for problem (2). The particular form of reaction term in (2) make impossible that analysis in the terms of Stuart-Watson method or two-time technique (Matkowsky) as they are presented in [20]. Consequently, we try to find a functional relationship between $u_{\max}$ (the maximum value of $\bar{u}(x)$ on $(0, L)$) and L. This turn out to be of the form $Lu_{\max} = const.$, which shows that indeed the bifurcation appears at infinity from the null solution. In fact the problem (2) is autonomous, and when one attempts to solve it in a closed form, encounters an integrand of the form $1/\sqrt{1 - t^4}$. We estimate subsequent integrals using a generalized mean value theorem suggested in [17].

The second aim of our paper is a direct approximation of the positive solution $\bar{u}(x)$ of (2) which satisfies (3). In this respect we built up a functional defined on $H_0^1(0, L)$ which has a positive lower bound. This functional is then augmented introducing the restriction (3) by means of Lagrange's multiplier method. Eventually, we determine the corresponding Euler's equations for this new functional and use them to obtain the finite elements approximation to $\bar{u}(x)$. Thus, it is underlined the importance of the conserved integral condition (3) in the numerical analysis of reaction-diffusion problem (2).

The content of the paper is as follows: in Section 2 we display some information on the existence and uniqueness of the positive solution $\bar{u}(x)$ of (2). We obtain the condition (4) and review some properties of $\bar{u}(x)$, including the bifurcation from infinity.

In section 3 we give the variational characterization of the positive solution and obtain the numerical approximation $\bar{u}_h(x)$ of $\bar{u}(x)$ by piecewise linear finite elements. We proceed as usually in f.e.m., write down the discrete analogous (18) of (2) and solve the resulting nonlinear algebraic system by Newton's method with initial guess satisfying (3).

2. SOME PROPERTIES OF $\bar{U}(X)$

In his paper [11], Laetsch considers a problem of type (2) with a more general reaction term. Specifically, he puts instead of u^p, $\lambda f(u)$, with $f(0) = 0$ and $f(w)/w$ is a non-decreasing function of w for $w > 0$. Then the problem (2) has exactly one positive solution for $\lambda > 0$ and as λ increases from 0, the norms of the corresponding solutions decreases from $+\infty$ to 0. He reduced the problem of solving (2) to a quadrature and observed that all positive solutions of (2), for $\lambda > 0$ are strictly positive and have exactly one maximum on $(0, L)$. They are also symmetric about the point $x = L/2$.

With these we can prove easy [6] the conditions (3) and (4). Multiplying the differential equation in (2) with $p = 3$ by $2u'(x)$, we write it in the form

$$\left[\left(u'(x)\right)^2\right]' = -\tfrac{1}{2}\left(u^4(x)\right)' \tag{5}$$

If we integrate (5) from 0 to x, $0 < x < L$, we get the first integral

$$u'(x)^2 - u'(0)^2 = -\tfrac{1}{2}u(x)^4,$$

or explicitly

$$u'(x) = \pm\tfrac{1}{\sqrt{2}}\sqrt{\left(\sqrt{2}u'(0)\right)^2 - u(x)^4}. \tag{6}$$

For the maximum value $u_{\max}$ of $u(x)$ on $(0, L)$ we have from the first integral

$$u_{\max}^2 = \sqrt{2}u'(0). \tag{7}$$

From (6) and (7) we deduce

$$\begin{aligned}\int_0^L u(x)\,\mathrm{d}x &= \int_0^L \frac{u\mathrm{d}u}{\frac{\mathrm{d}u}{\mathrm{d}x}} = 2\cdot\tfrac{1}{2}\int_0^{u_{\max}} \frac{\sqrt{2}\mathrm{d}u^2}{\sqrt{\left(\sqrt{2}u'(0)\right)^2-(u^2)^2}} \\ &= \sqrt{2}\arcsin\left.\frac{u^2}{\sqrt{2}u'(0)}\right|_0^{u_{\max}} = \frac{\pi}{\sqrt{2}}.\end{aligned}$$

We can apply the same strategy for the reaction term $f(u) = u^p$, $p > 1$, to obtain (4).

The nondimensional form of problem (2) for $p = 3$ reads as follows:

$$\begin{cases}\theta'' + \lambda^2\theta^3 = 0, & 0 < t < 1,\\ \theta(0) = \theta(1) = 0,\end{cases} \tag{8}$$

where $u_m := \max_{x\in[0,L]} u(x), \lambda := Lu_m$ and $t := x/L$.

As the differential equation in (8) is autonomous, usual manipulations and boundary condition in 0 imply:

$$t = \frac{\sqrt{2}}{\lambda}\int_0^{\theta}\frac{\mathrm{d}s}{\sqrt{1-s^4}}, \qquad t\in(0,\tfrac{1}{2}),\ \theta\in(0,1). \tag{9}$$

Here we used tacitly the symmetry of the positive solution about the middle of the interval. To approximate the integral in (9) we use the extension of the mean value theorem for integral suggested in [17]. Thus, there exists θ_t, such that

$$t = \frac{\sqrt{2}}{\lambda}\frac{\theta}{\sqrt{1-\theta_t^4}}, \tag{10}$$

where $0<\theta_t<\theta, \lim_{\theta\to 0}\theta_t/\theta = 1/(r+1)^{1/r}$, for $-1<r<0$ for which $\lim_{s\to 0} 1/(s^r\sqrt{1-s^4}) = 0$. and observe that $\theta_t = \mathcal{O}(\theta)$, as $\theta\to 0$ and $0<R<1$. If, motivated by the above asymptotics, we substitute $R\theta$ for θ_t in (10), we obtain the following approximation of the positive (and negative) solution of (8):

$$\theta(t) = \frac{\pm t}{\sqrt{\frac{1}{\lambda^2}+\sqrt{\frac{1}{\lambda^4}+t^4R^4}}}. \tag{11}$$

in an arbitrary small neighborhood of $t=0$.

Notice that the representation (11) retains all particularities of the exact solution of (8): the symmetry, the smoothness and the asymptotics properties near the boundary points. This entitles us to assimilate the behavior of $\theta'(0)$ obtained from (11) with that corresponding to exact solution. In fact we get

$$Lu_m = \theta'(0)\sqrt{2}. \tag{12}$$

But from [6], as an intermediate result, $\theta'(0)$ does not depend on L. Thus (12) means our bifurcation relationship. Thus, in the lack of a coherent strategy to study bifurcation from infinity we have considered the above *ad-hoc* method.

Remark 1. There do exist some literature gathered around the subject of existence, uniqueness, bifurcation and stability of solutions of (1). Thus, in his work [12], Matkowsky considers the stability of the null solution by asymptotic methods. He imposes on the reaction term $f(u)$ some technical conditions and avoids computational difficulties when takes into account only this solution. In the works of Ambrosetti and Rabinowitz [1], Aronson and Weinberger [2], Crandal and Rabinowitz [3],[4], Keller and Cohen [9], Simpson and Cohen [18], Sattinger [14], [15], [16] and Turner [19], to quote but a few, the authors take the advantage of a linear term in the full reaction term $f(u)$. Consequently, these analyses are useless for our purposes. □

3. THE VARIATIONAL CHARACTERIZATION OF THE POSITIVE SOLUTION

As is apparent from [6], some solvers contributed to a considerable insight into the nature of the solutions of (2). They used exclusively direct manipulation of the equation. With respect to the positive solution, a more penetrating discussion requires to study of an appropriate variational problem whose solution must satisfy (2) and (3).

The obvious choice, namely, the variational problem

$$\text{(V1)}\qquad \text{find } u \in H_0^1(0,L),\quad \int_0^L \Big(u'v' - u^3 v\Big)\,\mathrm{d}x = 0,\quad \forall v \in H_0^1(0,L),$$

of which (2) represents the Euler's equation, proves to be utterly unsuitable for our purposes. The main reason is that, the family of extremals of this problem which pass through a point $(0,0)$ for definiteness, do not form a field, and consequently, the classical sufficient criteria for the existence of extrema, due to Jacobi, become unapplicable (see [5, ch. 8]). We have to notice at this point that we have failed in our attempt to show that the functional

$$J_1(v) := \int_0^L ((v')^2 - v^4)\mathrm{d}x,\quad J_1 : H_0^1(0,L) \to \mathbb{R},$$

has a positive minimum.

Instead, using an idea from [13], we introduce the following generalized Rayleigh quotient (functional)

$$J : H_0^1(0,L) \to \mathbb{R},\quad J(v) := \left(\int_0^L (v')^2 \mathrm{d}x\right)^2 \Bigg/ \int_0^L v^4 \mathrm{d}x\ , \tag{13}$$

and prove the following result.

Lemma 1. *The functional $J(v)$ defined in* (13) *has a positive lower bound on $H_0^1(0,L)$.*

Proof. Recall that for any $y \in H_0^1(0,L)$ the Poincaré's inequality affirms that

$$\pi^2 \int_0^L y^2 \mathrm{d}x \le L^2 \int_0^L (y')^2 \mathrm{d}x.$$

For $y(x) = v^2(x)$, this implies another useful inequality

$$\pi^2 \int_0^L v^4 \mathrm{d}x \le (2L)^2 \int_0^L (vv')^2 \mathrm{d}x \tag{14}$$

Cauchy-Schwarz inequality, the left hand side boundary condition, and the inequality (14), enable one to write successively:

$$v^2(x) = \left(\int_0^x v'(t)\mathrm{d}t\right)^2 \le x \int_0^x (v')^2\,\mathrm{d}t < L \int_0^L (v')^2\,\mathrm{d}t,$$

$$\left(\tfrac{\pi}{2L}\right)^2 \int_0^L v^4 \mathrm{d}x \le L \int_0^L (v')^2 \left(\int_0^L (v')^2\,\mathrm{d}t\right)\mathrm{d}x = L\left(\int_0^L (v')^2\,\mathrm{d}x\right)^2.$$

This means that

$$J(v) \geq \left(\tfrac{\pi}{2}\right)^2 \tfrac{1}{L^3}, \quad \forall v \in H_0^1(0,L). \qquad \square$$

Our main result is concentrated in the following theorem.

THEOREM 2. *Given condition* (3), *a function* $u(x)$ *that extremizes the functional* $J(\cdot)$, *defined by* (13), *satisfies—for an appropriate choice of multiplier* μ*—the Euler's equation corresponding to the functional*

$$J^{**} : H_0^1(0,L) \to \mathbb{R}, \quad J^{**}(v) := J(v) + \mu \int_0^L v \mathrm{d}x.$$

Thus, the function $u(x)$ *and the multiplier* μ *can be determined from the system of equations*

$$\left\{ \begin{array}{l} \displaystyle\int_0^L (u'v' - u^3 v)\mathrm{d}x = \tfrac{\mu}{4} \int_0^L v \mathrm{d}x, \quad \forall v \in H_0^1(0,L), \\ \displaystyle\int_0^L u \mathrm{d}x = \tfrac{\pi}{\sqrt{2}}. \end{array} \right. \tag{15}$$

Proof. First, we observe that a function u that minimizes $J(\cdot)$ satisfies the necessary condition of extremum

$$\int_0^L \left((u')^2 - u^4 \right) \mathrm{d}x = 0. \tag{16}$$

In order to handle the condition (3) we have to introduce a new dependent variable $z(x)$ by $z(x) := \int_0^x u(s)\mathrm{d}s$, $z(0) = 0$, $z(L) = \frac{\pi}{\sqrt{2}}$ and $z'(x) = u(x)$. With this, consider the functional

$$J^* : H_0^1(0,L) \times H^1(0,L) \to \mathbb{R}, \quad J^*(v) := J(v) + \int_0^L \mu(x)(v(x) - z'(x))\mathrm{d}x,$$

for a sufficiently regular function $\mu(x)$.

The necessary conditions of extremum for J^* are

$$\left.\tfrac{\mathrm{d}J^*(u+\varepsilon v, z)}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} = 0 \quad \text{and} \quad \left.\tfrac{\mathrm{d}J^*(u, z+\eta y)}{\mathrm{d}\eta}\right|_{\eta=0} = 0.$$

The first one, in combination with (16), implies

$$\int_0^L (u'v' - u^3 v)\mathrm{d}x = \tfrac{1}{4} \int_0^L \mu(x) v(x) \mathrm{d}x, \quad \forall v \in H_0^1(0,L), \tag{17}$$

and the second one leads to

$$\int_0^L \mu(x) y'(x) \mathrm{d}x = 0, \quad \forall y \in H^1(0,L).$$

For sufficiently smooth $y \in H_0^1(0,L)$, such that the fundamental lemma of variational calculus apply, the last integral equality ensures that $\mu'(x) = 0$. Consequently, the Lagrange's multiplier μ reduces to a real parameter.

Thus, (17) and (3) imply (15). More than that,

$$\left.\tfrac{\mathrm{d}J^*(u+\varepsilon v, z)}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} = 0$$

means the first equation in the system (15). This completes the proof. □

We have to underline that all problems of extremum we have encountered are meant on the whole Sobolev space $H_0^1(0,L)$ equipped with the usual norm.

The positive solution $u(x)$ of the system (15) is a weak approximation to the positive solution $\bar{u}(x)$ of (2) and (3). To find numerically this approximation we discretize the equations in (15) using classical f.e.m.

The positive solution is approximated by

$$u_h(x) = \sum_{k=1}^{N} c_k \varphi_k(x),$$

where the piecewise linear function $\varphi_k(x)$ satisfies $\varphi_k(x_j) = 0$ for $k \neq j$ and $\varphi_k(x_k) = 1$, $x_k = kh$ for $k = 0, 1, \ldots, N+1$ and $h = L/(N+1)$.

For each N, u_h must be a solution of the discrete analogous of (15),

$$(18) \qquad \begin{cases} \int_0^L \left(u_h' \varphi_k' - u_h^3 \varphi_k\right) \mathrm{d}x = \frac{\mu}{4} \int_0^L \varphi_k \mathrm{d}x, & \text{for } k = 1, \ldots, N, \\ \int_0^L u_h \mathrm{d}x = \frac{\pi}{\sqrt{2}} \end{cases}$$

which becomes a nonlinear algebraic system, $F(c) = 0$, for the unknowns $c = (c_1, \ldots, c_N, \mu)$. Here $F = (F_1, \ldots, F_N, F_{N+1})$ and

$$(19) \qquad \begin{aligned} F_n(c) \;=\; & \tfrac{c_{n-1}}{h} - \tfrac{2c_n}{h} + \tfrac{c_{n+1}}{h} + \tfrac{c_{n-1}^3 h}{20} + \tfrac{c_{n-1}^2 c_n h}{10} + \tfrac{3c_{n-1} c_n^2 h}{20} \\ & + \tfrac{2c_n^3 h}{5} + \tfrac{3c_n^2 c_{n+1} h}{20} + \tfrac{c_n c_{n+1}^2 h}{10} + \tfrac{c_{n+1}^3 h}{20} + \tfrac{\mu}{4} h \end{aligned}$$

for $n = 1, \ldots, N$, where we put $c_0 = c_{N+1} = 0$, in order to impose the boundary conditions and

$$(20) \qquad F_{N+1}(c) = h \sum_{n=1}^{N} c_n - \tfrac{\pi}{\sqrt{2}}$$

We solve this nonlinear system by Newton's method. Starting with an initial guess of the form $c_k^0 = x_k(L - x_k)$, for $k = 1, \ldots, N$, and $\mu = 10$, Newton's method implies the following sequence of iterations by solving the sequence of linear systems

$$F'(c^\alpha)(c^{\alpha+1} - c^\alpha) = -F(c^\alpha), \text{ for } \alpha = 0, 1, \ldots .$$

This means that, for every α, we have to solve a linear algebraic system, until for a given ε, $\left\|c^{\alpha+1} - c^\alpha\right\| < \varepsilon$. In spite of that, the method is not so expensive because of the sparsity of the Jacobian $F'(c^\alpha) = \left(\frac{\partial F_i(c^\alpha)}{\partial c_k}\right)_{i,k=1,\ldots,N+1}$. We remark that whenever the f.e.m. is applied directly to the problem (2), i.e. the integral condition (3) is ignored, the attracting basin of the positive solution becomes very narrow. Consequently, Newton's method converges to the positive solution only for initial approximation $u_h^0(x)$ sufficiently close to this solution. That is why we have incorporated the integral condition (3) in the above algorithm. The numerical experiments with this (most of them reported in [7] confirm the fact that the attracting basin of the positive solution becomes larger. This underlines the importance of the integral condition (3) and furnishes an effective algorithm for the numerical computation of the positive solution to problem (2).

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