Spurious Behavior for a Numerical Scheme of Nonlinear Elliptic Equations

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In this paper we investigate finite difference approximations of nonlinear elliptic equations of the form $\Delta u + \lambda (u + u^p) = 0$ in three dimensions, where λ is a positive parameter. We show the existence of spurious solution branches, these solutions are spurious in the sense that they are not solutions of the differential problem. We also construct a modified problem describing the behaviour of numerical solutions, so the finite difference method may be regarded as an approximation of the modified problem. We present the results of some numerical experiments to substantiate our claims. © 1995 Academic Press, Inc.

1. INTRODUCTION

In this paper we investigate the performance of the finite difference methods when used to approximate the semilinear partial difference problem

$$\Delta u + \lambda f(u) = 0, \quad \text{in } \Omega,$$

 $u = 0, \quad \text{on } \delta\Omega.$ (1.1)

with u > 0 inside Ω ; Ω is a bounded regular domain in R^N (N > 2) with boundary $\delta\Omega$; Δ is the Laplacian, λ is a positive parameter, and f(u) is a superlineal function with polynomial grown. Let us recall that this type of problem arises in a variety of situations, in the theory of nonlinear diffusion generated by nonlinear sources, in quantum field theory and mechanical statistics, in plasma physic (see [15] for more references).

In particular we shall consider the special nonlinear function

$$f(u) = u + u^p, \quad p > 1.$$
 (1.2)

Problem (1.1), (1.2) has been the center of many analytical investigations. The analytical interest centres on the observation that for $p < p_c = (N+2)/(N-2)$, p_c is denominated by the critical Sobolev exponent, the space $H_0^1(\Omega)$ is compactly embedded into the space $L^{p+1}(\Omega)$ [1 or 5], and using the classical techniques based upon the calculus of variations, it is possible to deduce that (1.1), (1.2) has positive solutions for all values of $\lambda > 0$ [5, 15]. In contrast, when $p > p_c$ the embedding is

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not even continuous and these variational techniques break down and the number of solutions depends on the values of λ and p. It is quite interesting remark that the break down in the variational techniques as a means to solving (1.1), (1.2) is associated with a real change of the bifurcation diagram for solutions.

When $\Omega = B$ (unit ball), according to the results in Gidas, Ni, and Niremberg [6], all positive solutions of (1.1), (1.2) must be radially symmetric, and the problem reduces to the following ordinary differential equation problem

$$u_{rr} + \frac{N-1}{r}u_r + \lambda(u+u^p) = 0, \quad \text{in } 0 < r < 1,$$

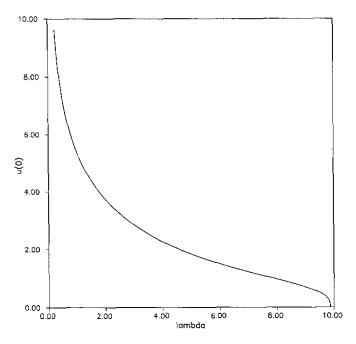
$$u_r(0) = u(1) = 0,$$
 (1.3)

where u(r) is a positive function of the radial distance. Moreover, from the maximum principle, the maximum of u is attained at the origin and it is known from Rabinowitz [19], that any solution with $p > p_c$ must have λ bounded away from zero.

For $p > p_c$ Budd and Norbury [4] have shown that for 2 < N < 10 there exists a value of λ^* such that (1.3) has a positive solution when $\lambda^* < \lambda < \lambda_1$, where λ_1 is the first eigenvalue of the linearized problem, and there exists $\lambda^* \in (\lambda^*, \lambda_1)$, where (1.3) has an infinite number of positive solutions. We illustrate these behaviours by giving four bifurcation diagrams where the solutions were continued in λ using the software package λ UTO. Figures 1 and 2 show the bifurcation diagrams for N = 3, p = 4 and p = 7, respectively (here the critical exponent is $p_c = 5$), and we can see very clearly the dramatic change in behaviour of the solutions. Figures 3 and 4 show the bifurcation diagrams in supercritical cases for p = 7 and the dimensions N = 5 and N = 10, as it seems they are more vertical as the dimension increases.

Murdoch and Budd [17] considered a convergence finite element approximation for (1.3) with N=3 and p>5, they showed the existence of apparently spurious solution branches. These solutions are spurious in the sense that instead of $\lambda \varepsilon (\lambda^*, \lambda_1)$ as the maximum norm become unbounded (Fig. 2), as λ approaches zero.

Many papers on spurious solutions have appeared in recent years. Brezzi, Ushiki, and Fujii [3] have found spurious invariant cycles in the Euler's method for a differential equation with



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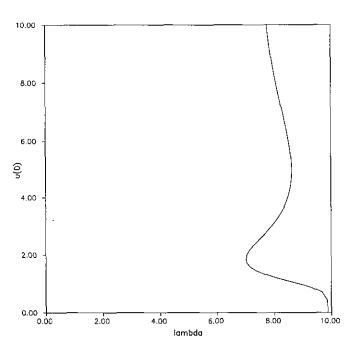
FIG. 1. AUTO, N = 3, p = 4.

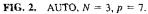
FIG. 3. AUTO, N = 5, p = 7

a Hopf bifurcation. Griffiths and Mitchell [8], Sleeman *et al.* [23], Mitchell and Schoombre [21], Schoombre [22], and Stuart [25] have found spurious periodic solutions in convergence methods for nonlinear reaction—diffusion equations. Iserles [12], (1990), Hairer, Iserles, and Sanz-Serna [10] Iserles, Peplow, and Stuart [13], Griffiths, Sweby, and Yee [9], and

Humphries [11] have studied the spurious solutions introduced by time discretisations.

The theme of this paper is the investigation of finite difference methods for (1.3) with spurious solution branches. The scheme study is simple but may be modified to cater to other methods with higher accuracy. The main idea is that (1.3) is not robust





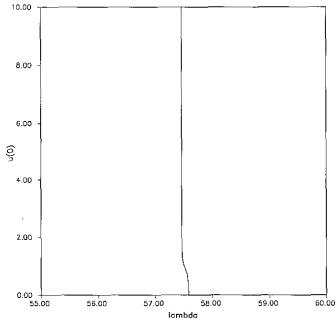


FIG. 4. AUTO, N = 10, p = 7.

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in the sense of Strikwerda [24], so the qualitative behaviour of the solution is affected by the addition of lower order terms or small changes in the coefficients. If the problem is not robust, then the construction of different schemes of it will be more difficult and our finite difference method may be regarded as an approximation of the modified problem [7] that aims at describing the behaviour of the numerical solutions of our numerical experimentations. Roughly speaking, the problem is structurally unstable and small perturbations may affect seriously the qualitative behaviour of the solutions.

The layout of this paper is as follows. In Section 2 we construct and study the explicit scheme for (1.3). In Section 3 we demonstrate that there exist spurious solutions and we also provide numerical results to show that these spurious solutions approach zero, and finally in Section 4 we construct the modified problem describing the behaviour of the numerical solutions.

2. THE FINITE DIFFERENCE METHOD

In order to discretize (1.3), we subdivide [0, 1] into M + 1 equal subintervals,

$$r_i = ih$$
, $i = 0, 1, ..., M + 1$, $h = \frac{1}{M+1}$,

and with the abbreviation $U_i \simeq u(r_i)$ we replace the differential quotients u_{rr} and u_r by the second difference quotients

$$u_{rr}(r_i) \simeq \frac{U_{i+1} - 2U_i + U_{i-1}}{h^2},$$

 $u_{rr}(r_i) \simeq \frac{U_{i+1} - U_{i-1}}{2h}.$

The values U_i satisfy the equations

$$\frac{1}{h^2} \cdot (U_{i+1} - 2U_i + U_{i-1}) + \frac{N-1}{2ih^2} \cdot (U_{i+1} - U_{i-1})
+ \lambda \cdot (U_i + U_i^p) = 0,$$
(2.1)

i=1, ..., M. With the boundary conditions $U_{M+1}=0$ and $U_0=U_1$ from the boundary conditions of (1.3), the vectors $\mathbf{U}=(U_1, ..., U_M)^{\mathrm{T}}, \mathbf{U}^p=(U_1^p, ..., U_M^p)^{\mathrm{T}}$, and the $M\times M$ matrix

$$A_{N}^{h} = \begin{pmatrix} \frac{3-N}{2} - 2 & 1 + \frac{N-1}{2} \\ 1 - \frac{N-1}{4} & -2 & 1 + \frac{N-1}{4} \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots & 1 + \frac{N-2}{2(M-1)} \\ & & & 1 - \frac{N-1}{2M} & -2 \end{pmatrix}, (2.2)$$

where the subscript N and the superscript h indicate that A_N^h depends on the mesh-size h and the dimention N, Eqs. (2.1) are equivalent to

$$\frac{1}{h^2} \cdot A_N^h \cdot \mathbf{U} + \lambda \cdot (\mathbf{U} + \mathbf{U}^p) = \mathbf{0}. \tag{2.3}$$

We first want to show some properties of the matrix A_N^h .

LEMMA 2.1. For $N \leq 5$.

- (i) The matrix A_N^h is irreducibly diagonally dominant.
- (ii) The matrix A_N^h is nonsingular.
- (iii) The real parts of eigenvalues of A_N^h are negative.

Proof. (i) Simple calculations lead us to the result.

(ii) and (iii) are direct consequences of (i) and Theorem 1.8 of Vargas [26, 23],

Remark. For higher dimension problems $N \ge 6$, the second row of A_N^h does not satisfy the diagonal dominance condition, and conclusion (i) is uncorrect, however, the numerical evidences show that (ii) and (iii) are true. So, in the opinion of the author, the restriction $N \le 5$ is only a technical condition in order to demonstrate (ii) and (iii).

LEMMA 2.2. For $N \leq 5$, the matrix $(A_N^h)^{-1}$ is negative.

Proof. Let be $(A_N^h)^{-1} = (\mathbf{x}_1, ..., \mathbf{x}_M)$, where the vector $\mathbf{x}_i = (x_1, ..., x_{M,i})^T$ is the *i*th column of the matrix $(A_N^h)^{-1}$. Then

$$A_N^h \cdot \mathbf{x}_i = \mathbf{e}_i, \quad i = 1, ..., M, \tag{2.4}$$

with $\mathbf{e}_i = (0, ..., 0, 1, 0, ..., 0)^T$ as the *i*th coordinate vector.

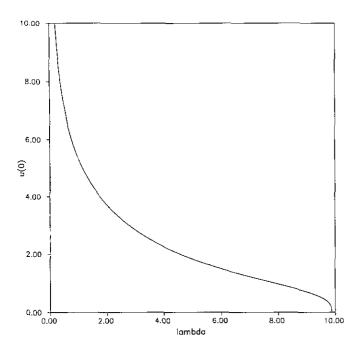


FIG. 5. PITCON, N = 3, p = 4, $h = \frac{1}{100}$.

For i = 1, because the first equation of (2.5) is

$$\frac{N+1}{2} \cdot (-x_{1,1} + x_{2,1}) = 1,$$

it follows that $x_{1,1} < x_{2,1}$. From the second equation,

$$0 = \left(1 - \frac{N-1}{4}\right) \cdot x_{1,1} - 2x_{2,1} + \left(1 + \frac{N-1}{4}\right) \cdot x_{3,1}$$

$$< \left(1 + \frac{N-1}{4}\right) \cdot (x_{3,1} - x_{2,1}),$$

we obtain

$$x_{1,1} < x_{2,1} < x_{3,1}$$
.

Therefore using M-1, we obtain

$$x_{1,i} < x_{2,i} < \cdots < x_{M-1,i} < x_{M,i}$$

and finally we use

$$0 = \left(1 - \frac{N-1}{2M}\right) \cdot x_{M-1,1} - 2x_{M,1} < \left(-1 - \frac{N-1}{2M}\right) \cdot x_{M,1}$$

to obtain

$$x_{1,1} < x_{2,1} < \cdots < x_{M-1,1} < x_{M,1} < 0.$$

A similar procedure shows that for any i > 1, the components of \mathbf{x}_i satisfy

$$x_{1,i} = x_{2,i} = \dots = x_{i,i} < x_{i+1,i} < \dots < x_{M,i} < 0,$$
 (2.5)

which concludes the proof.

We shall now derive the basic properties of the matrix – $(A_N^h)^{-1}$ by using the Perron–Frobeniu's theorem [26].

THEOREM 2.3, For $N \leq 5$

- (i) $-(A_N^i)^{-1}$ has a simple positive eigenvalue μ_1^h equal to its spectral radius.
 - (ii) To μ_1^h there corresponds an eigenvector $\varphi_1^h > 0$.

In order to study the convergence we consider the nonlinear operator equation

$$\Phi_h(\mathbf{U}) = \frac{1}{h^2} \cdot A_N^h \cdot \mathbf{U} + \lambda \cdot (\mathbf{U} + \mathbf{U}^p), \tag{2.6}$$

Assume that the solution possesses bounded derivatives; obviously (2.1) approximates (1.3) with second-order accuracy, but the approximation of the boundary condition is first order only. Hence the numerical scheme (2.3) is consistent with the differential problem (1.3) for N=3 and its accurate order is one.

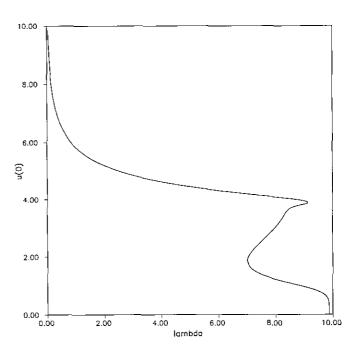


FIG. 6. PITCON, N = 3, p = 7, $h = \frac{1}{2000}$

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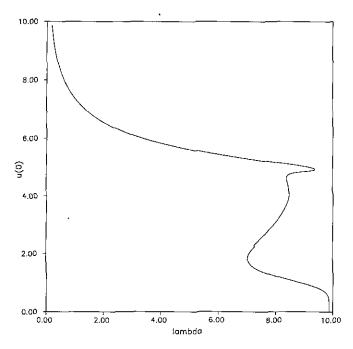


FIG. 7. PITCON, N = 3, p = 7, $h = \frac{1}{400}$.

To study the stability, we must be used the results of Lopez-Marcos and Sanz-Serna [16] and Sanz-Serna [20], where the method is stable with thresholds depending on the discretization parameter. Murdoch and Budd have applied this idea for Galerkin approximations to (3.1) and they have proved that the spurious solutions lie outside the stability ball centred on the zero solution. This theory would need an introduction to the

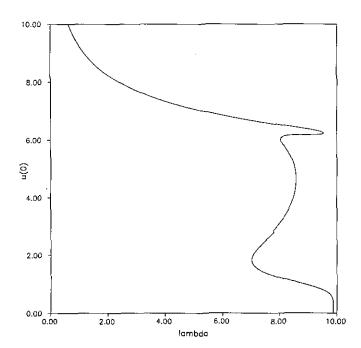


FIG. 8. PITCON, N = 3, p = 7, $h = \frac{1}{800}$.

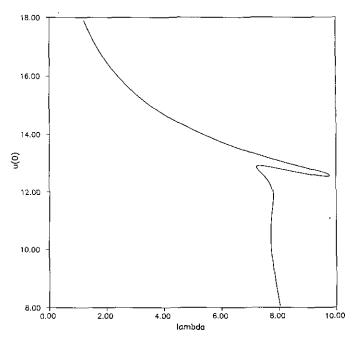


FIG. 9. PITCON, N = 3, p = 7, $h = \frac{1}{6400}$.

discretization framework which exceeds the scope of this article.

The linearized discretization

$$(\mathbf{\Phi}_h)_u(\mathbf{U}) = \frac{1}{h^2} \cdot A_N^h + \lambda \cdot (1 + p \cdot U_j^{p-1}) \cdot I \tag{2.7}$$

is locally Lipschitz continuous, and then the linearized stability is equivalent to the stability with some suitable (h-dependent) thresholds. The stability ball must act to separate the convergent and the spurious solutions.

3. SPURIOUS SOLUTIONS

In this section we shall demonstrate that there exist spurious solutions in (2.3) in the sense that $\lambda \to 0$ as they become unbounded in the maximum norm.

Because there exists $(A_N^h)^{-1}$ for $N \le 5$, we can write (2.3) in the form

$$\mathbf{U} = \lambda L_N^h \cdot \mathbf{U} - \lambda h^2 \cdot (A_N^h)^{-1} \mathbf{U}^p, \tag{3.1}$$

where $L_N^h = -h^2$. $(A_N^h)^{-1}$ and we now consider its branches of solutions (λ, \mathbf{U}) of $R \times R^M$ with fixed h and allow λ to vary.

It is well known from the standard bifurcation theory that the curve of trivial solutions $(\lambda, 0)$, has a bifurcation point when λ is characteristic value of L_N^h of odd multiplicity [18]. Here the characteristic values of L_N^h are $\lambda_i^h = 1/h^2 \mu_i^h$, where μ_i^h is eigenvalue of $-(A_n^h)^{-1}$ and the smaller of them corresponding to the bigger eigenvalue of $-(A_N^h)^{-1}$,

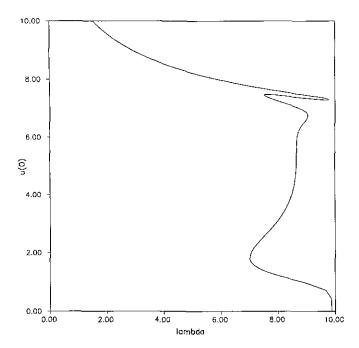


FIG. 10. AUTO, mod $h = \frac{1}{100}$.

$$\lambda_1^h = 1/h^2 \, \mu_1^h. \tag{3.2}$$

The following theorem is a direct consequence of the classical global bifurcation theory [18].

THEOREM 3.1. (i) The problem (3.1) has a branch of solutions Γ_1^h such that $(\lambda_1^h, \mathbf{0}) \in \Gamma_1^h$, and Γ_1^h meets other bifurcation point $(\lambda_j^h, \mathbf{0})$ with $j \neq 1$ or is unbounded in the norm $|\lambda| + ||\mathbf{U}||_{\infty}$.

(ii) As $\lambda \to \lambda_1^h$ the first eigenvalue of L_N^h , $\mathbf{U} = \alpha \cdot \varphi_1^h + \mathbf{o}(\alpha)$ for $\alpha > 0$ near zero.

We shall now derive some properties of the branch of solutions Γ_1^h . These are contained in the following theorem.

THEOREM 3.2. If $(\lambda, \mathbf{U}) \in \Gamma_1^h$ then

- (i) $0 \le \lambda \le \lambda^h$.
- (ii) $U_i > 0$, i = 1, ..., M.

Proof. (i) If $(\lambda, \mathbf{U}) \in \Gamma_1^h$ is in the neighbourhood of $(\lambda_1^h, \mathbf{0})$, (λ, \mathbf{U}) satisfies (3.1), and $\mathbf{U} = \alpha \varphi_1^h + \mathbf{o}(\alpha)$, then

$$\alpha \varphi_1^h + \mathbf{o}(\alpha) = \lambda L_N^h \cdot (\alpha \varphi_1^h + \mathbf{o}(\alpha)) - \lambda h^2 \cdot (A_N^h)^{-1} (\alpha \varphi_1^h + \mathbf{o}(\alpha))^p;$$

therefore

$$\alpha \varphi_1^h = \alpha \lambda L_N^h \varphi_1^h - \lambda h^2 (A_N^h)^{-1} \alpha^p (\varphi_1^h)^p + \mathbf{o}(\alpha). \tag{3.3}$$

On the other hand,

$$\alpha \varphi_1^h = \alpha \lambda_1^h L_N^h \varphi_1^h, \tag{3.4}$$

and subtracting (3.4) and (3.3) gives

$$\mathbf{0} = \alpha(\lambda - \lambda_1^h) L_N^h \varphi_1^h - \lambda h^2 (A_N^h)^{-1} \alpha^p (\varphi_1^h)^p + \mathbf{o}(\alpha). \tag{3.5}$$

Since $-\lambda h^2 (A_N^h)^{-1} \alpha^p (\varphi_1^h)^p$ is positive, we immediately conclude from (3.5) that $\lambda < \lambda_1^h$.

In order to demonstrate that $\lambda > 0$ it will be sufficient for $\lambda \neq 0$ because $\lambda_1^h > 0$.

Let's suppose that $\lambda = 0\varepsilon\Gamma_1^h$; from (3.1) $\mathbf{U} \equiv \mathbf{0}$ and then (0, $\mathbf{0})\varepsilon\Gamma_1^h$ and it would be a bifurcation point of (3.1), which is a contradiction.

(ii) Let be $(\lambda^*, \mathbf{U}^*) \varepsilon \Gamma_1^h$ such that $U_k^* \le 0$ and $U_j^* > 0$ for all $j \ne k$. From the continuity of \mathbf{U} with respect λ , there must exist λ between λ^* and λ_1^h , where $U_k = 0$ and $U_j \ge 0$ for all $i \ne k$.

If k = 1, the first equation of (3.1),

$$\frac{N+1}{2} \cdot (U_2 - U_1) + \lambda h^2 U_1 + \lambda h^2 U_1^p = 0,$$

implies $U_2 = 0$ and, similarly, $U_3 = \cdots = U_M = 0$, which is not possible.

If k > 1, the kth equation is

$$\left(1 - \frac{N-1}{2k}\right) \cdot U_{k-1} + \left(1 + \frac{N-1}{2k}\right) \cdot U_{k+1} = 0,$$

since for $N \le 5$ the coefficients are positive. Then $U_{k-1} = U_{k-1} = 0$ and so on, U = 0, which is again a contradiction.

Moreover, simple calculations lead us to the discrete maximum principle.

Corollary 3.3. If $(\lambda, \mathbf{U}) \in \Gamma_1^h$ then $U_1 > U_2 > \cdots > U_u > 0$.

We now consider the first equation of algebraic system (3.1)

$$\frac{N+1}{2} \cdot (-U_1 + U_2) + \lambda h^2 \cdot (U_1 + U_1^p) = 0,$$

since by the corollary above

$$\lambda h^2 \cdot (1 + U_1^{p-1}) < \frac{N+1}{2} = K,$$

then

$$U_1 < \sqrt[r-1]{K/\lambda h^2} - 1, \tag{3.6}$$

and we deduce the following important result.

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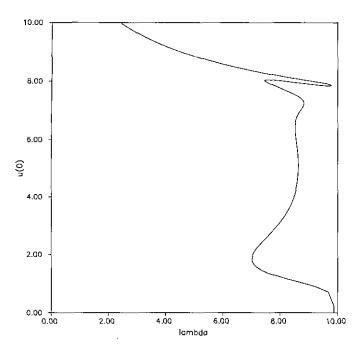


FIG. 11. AUTO, mod $h = \frac{1}{200}$.

Theorem 3.4. The curve Γ_1^h tends to infinity as $\lambda \to 0$.

The conclusion of Theorem 3.4 is totally different from the known behaviour of the solution described in Section 1 for $p > p_c$; here $U_1 \to \infty \Rightarrow \lambda \to 0$ and, consequently, it is quite possible to obtain spurious solutions. Now we present numerical results to substantiate our claims.

Figure 5 is the bifurcation diagram obtained for the algebraic system (3.1) with N=3, p=4 (subcritical exponent) and $h=\frac{1}{100}$, using the software package PITCON. It is clear from Figs. 1 and 5 that our finite difference method provided a good approximation to the solution.

On the other hand, for the case p = 7 (supercritical exponent) and using again the package PITCON we obtain the bifurcation diagrams for different mesh spacing h, they are shown in the Figs. 6 through 9. From the bifurcation diagrams it is clear that the numerical method has a branch of solutions such that $\lambda \to 0$ as $\|\mathbf{U}\|_{\infty} \to \infty$, which is different from the correct solution and were advertised by Theorem 3.4. Moreover, as the mesh spacing is reduced, more and more of the structure of the bifurcation diagram is resolved.

4. THE MODIFIED PROBLEM

The modified equation technique for the analysis of a numerical scheme consists of the construction of a modified differential equation such that the numerical solutions are more accurately matched by the solutions of the modified equation than by the solutions of the original differential equation being solved by the numerical scheme. It should be observed that although it is customary in the literature to talk about modified equations, it is essential to consider modified problems, because the modified equation should be supplemented by the necessary initial or boundary conditions [7].

In order to construct a modified problem here, we observe that (2.1) approximates the differential equation of (1.3) with second-order accuracy, while $U_0 - U_1 = 0$ is only a first-order accurate replacement of boundary condition $u_r(0) = 0$. However, $U_0 = U_1$ is a second-order accurate replacement of new boundary condition $u_r(0) + (h/2) u_{rr}(0) = 0$ which depends on h and $u_{rr}(0)$. To remove $u_{rr}(0)$ we consider that because $u_r/r \to u_{rr}$ as $r \to 0$, consequently the differential equation is $N \cdot u_{rr} + \lambda(u + u^p) = 0$ as $r \to 0$ and the problem

$$v_{rr} + \frac{N-1}{r}v_{r} + \lambda(v + v^{p}) = 0,$$

$$v(1) = 0,$$

$$v_{r}(0) - \frac{\lambda h}{2N}(v(0) + v(0)^{p}) = 0,$$
(4.1)

appears to be a good candidate for the role of the modified problem with second-order of correctness, and we claim that the numerical solution U is a better approximation to v(r) than u(r). Now we present numerical results to substantiate this claim.

Figures 10 and 11 are the bifurcation diagrams of (4.1) using again the software package AUTO for N=3, p=7, and $h=\frac{1}{100}$, $h=\frac{1}{200}$, respectively. We can see branches of solutions such that $\lambda\to 0$ as $\|v\|_\infty\to\infty$, describing the behaviour of the numerical solution (let us compare, for example, Fig. 8 with Fig. 10 or 11); then we conclude that the modified problem (4.1) provides a valid description of the numerical solutions. And when we are trying to resolve (1.3), in fact, we are approximating the modified problem with important qualitative changes in the behaviour of the branches of the solutions.

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