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Nonlinear Boundary Value Problems Suggested By Chemical Reactor Theory*

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1. INTRODUCTION

This paper was motivated by a certain nonlinear boundary value problem which has recently arisen in the theory of tubular chemical reactors. We shall treat it and some mathematical generalizations of it here.

Specifically we shall be concerned with (i) establishing the existence of a unique *positive* solution of the nonlinear boundary value problem

$$Lu = -f(x, u), \quad x \in D, \tag{1.1}$$

$$Bu = 0, \quad x \in \partial D, \tag{1.2}$$

(ii) characterizing this solution by constructive methods, and (iii) deriving pointwise upper and lower bounds on this solution. Here $x = (x_1, ..., x_m)$ and L is the uniformly elliptic second-order operator

$$Lu = \sum_{i,j=1}^{m} a_{ij}(x) \frac{\partial^2 u}{\partial x_i \, \partial x_j} + \sum_{j=1}^{m} a_j(x) \frac{\partial u}{\partial x_j} - a_0(x)u, \tag{1.3}$$

on a bounded domain D, the coefficients $a_{ij}(x)$, $a_j(x)$ are Hölder continuous in $\bar{D}$, $a_0(x) \geq 0$ is Hölder continuous, and for all unit vectors $\xi = (\xi_1, ..., \xi_m)$,

$$\sum_{i,j=1}^{m} a_{ij}(x)\, \xi_i \xi_j \geq a > 0, \qquad x \in D. \tag{1.4}$$

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The boundary conditions (which we write briefly as $Bu = 0$) will be taken as

$$\alpha(x)\, u(x) + \frac{\partial u}{\partial n}(x) = 0, \qquad x \in \Gamma_1,$$
$$u(x) = 0, \qquad x \in \Gamma_2, \tag{1.5}$$

where Γ_1 and Γ_2 are disjoint subsets of the C^2-boundary ∂D of D, with $\Gamma_1 \cap \Gamma_2 = \partial D$, $\partial/\partial n$ is the outer conormal derivative on Γ_1, and $\alpha(x)$ is nonnegative and continuous for $x \in \Gamma_1$. Either Γ_1 or Γ_2 may be empty; however, if Γ_2 is empty, we require that either $\alpha(x)$ or $a_0(x)$ is not identically zero.

Markus and Amundson [2] have studied the following autonomous ordinary differential two-point boundary value problem which is a special case of (1.1), (1.2):

$$w''(y) + Aw'(y) + Bf(w) = 0, \qquad 0 \leqslant y \leqslant 1, \tag{1.6}$$

$$w'(0) = 0, \tag{1.7}$$

$$w'(1) + Aw(1) = 0. \tag{1.8}$$

The function w represents the dimensionless temperature in a tubular reactor of length 1 in which there is occuring a single exothermic homogeneous chemical reaction involving several chemical species. A and B are known constants, and the function $f(w)$, which essentially represents the rates of chemical production of the species, is a smooth function increasing from $f(-1) = 0$ to a maximum at some point y_m (which may be positive or negative) and decreasing thereafter to become zero at some $c > y_m$. The concentrations of the various chemical species involved in the reaction can be determined easily from a knowledge of w and the stoichiometric coefficients of the species. In the light of this interpretation of (1.6), (1.7), (1.8) we are led to impose the following conditions on the nonlinearity f in (1.1):

H-1: $f(x, u)$ is Hölder continuous in (x, u) and continuously differentiable with respect to u for $x \in \bar{D}$ and all $u \geqslant 0$.

H-2: $f(x, 0) > 0$ and $f(x, c) = 0$ for all $x \in D$. Here c is a fixed positive constant.

H-3: $f(x, u) < 0$ on $u \geqslant c$.

H-4: $(\partial/\partial u)[f(x, u)/u] < 0$ on $\bar{D}$ for $0 < u \leqslant c$.

H-5: $f_u(x, u) \geqslant 0$ on $0 \leqslant u < b$ and $f_u(x, u) \leqslant 0$ on $b < u \leqslant c$. Here b is a fixed nonnegative constant; i.e., $b \geqslant 0$.

Condition H-4 is a concavity condition which implies that $f(x, u)$, when graphed as a function of u for fixed x, has the property that any line segment from the origin to the function lies below the graph of the function. In addition, condition H-2 together with H-4 imply that, for fixed x, the tangent to the curve $y = f(x, u)$ on $0 < u \leqslant c$ intersects the axis of ordinates (i.e., the $u = 0$ axis) in $y > 0$. These geometrical properties have been enlightening to us in the investigation of related problems (see [3]–[5]); they shall play a role in our analysis here.

In Section 2 we establish a priori bounds on solutions of (1.1), (1.2) by using several results which follow from the strong maximum principle for uniformly elliptic second order equations. The specific consequences of the maximum principle which we utilize have been stated and used by Keller [6] for problems similar to ours.

In Sections 3 and 4 we prove existence and uniqueness of a *positive* solution of (1.1), (1.2), respectively. We introduce iteration procedures, defined by solutions of *linear* equations, which "pinch" the positive solution in the sense that one sequence converges monotonically to this solution from above while another sequence converges monotonically to this solution from below. Thus, in a given problem, for example, we can obtain pointwise upper and lower bounds on the solution with the assurance that the bounds become more accurate with each iterate.

Our iteration procedure is patterned after that used by Keller [6] who, in fact, has studied problems of a more general nature than ours. In order to achieve our more specific results we have limited our attention to the type of nonlinearity $f(x, u)$ which arises when we interpret the problem (1.1), (1.2) as that of finding the generalized temperature in an n-dimensional chemical reactor of arbitrary size and shape.

2. A Priori Bounds

The rough bounds which we obtain in this section are consequences of several results which follow from the strong maximum principle [1] for uniformly elliptic second order equations. More precisely, we shall use the following theorem which is stated and proved in this form in the previously mentioned work of H. B. Keller:

THEOREM 2.1. *If* $\phi(x) \in C^1(\bar{D}) \cap C^2(\bar{D})$ *and satisfies for some constants* $M_1 \geqslant 0$ *and* $M_2 \geqslant 0$

$$L\phi(x) \geqslant 0 \text{ on } D_1 \cap D, \text{ where } D_1 \equiv \{x \mid x \in \bar{D}, \phi(x) \geqslant M_1\}$$

and

$$B\phi(x) \leqslant 0 \text{ on } \partial D_2 \equiv \{x \mid x \in \partial D, \phi(x) \geqslant M_2\},$$

then

$$\phi(x) \leqslant M_0 \equiv \max(M_1, M_2) \text{ for all } x \in \bar{D}.$$

Taking $M_1 = M_2 = c$, it immediately follows as a consequence of this theorem that we have the

THEOREM 2.2. *Let $f(x, u)$ satisfy* H-1 *to* H-3. *Then every positive solution $u(x)$ of* (1.1), (1.2) *satisfies*

$$0 \leqslant u(x) \leqslant c. \tag{2.1}$$

The a priori bounds (2.1) can be used to replace the problem (1.1), (1.2) by an equivalent one in which $f(x, u)$ has any desired properties for $u < 0$ and $u > c$. *For the purposes of the present paper this shall always consist of replacing $f(x, u)$ by $f^*(x, u)$ defined as*

$$f^*(x, u) = \begin{cases} f_u(x, 0)\, u + f(x, 0) & \text{if} \quad u < 0 \\ f(x, u) & \text{if} \quad 0 \leqslant u \leqslant c \\ f_u(x, c)\, u + [f(x, c) - f_u(x, c)c] & \text{if} \quad u > c. \end{cases} \tag{2.2}$$

Equation (2.2) states that we retain $f(x, u)$ in $0 \leqslant u \leqslant c$ and continue $f(x, u)$ into $u < 0$ and $u > c$ by its tangent line at $u = 0$ and $u = c$, respectively. *We now state once and for all that throughout the remainder of this paper we are replacing $f(x, u)$ in* (1.1) *by $f^*(x, u)$ defined by* (2.2).

3. EXISTENCE OF POSITIVE SOLUTIONS AND SHARP BOUNDS

Under conditions H-1 to H-4 we shall now show that the boundary value problem (1.1), (1.2) has positive solutions. (Note that since $u(x) \equiv 0$ is not a solution of (1.1), (1.2), then positive solutions can not vanish identically.)

In order to establish this we shall need the following Positivity Lemma which is essentially the strong maximum principle for elliptic equations (see [1] for a proof in this form):

POSITIVITY LEMMA. *Let $\phi(x)$ be twice continuously differentiable and satisfy*

$$L\phi \leqslant 0, \quad x \in D,$$
$$B\phi = 0, \quad x \in \partial D.$$

Then, either $\phi(x) \equiv 0$ on $\bar{D}$ or $\phi(x) > 0$ for $x \in D$.

Since f and f_u are bounded on $u \geqslant 0$, we can find a *positive* Hölder continuous function $M(x)$ and a *negative* Hölder continuous function $\Omega(x)$ such that

$$M(x) \geqslant f(x, u), \qquad \text{for} \quad x \in D,\ u \geqslant 0, \tag{3.1}$$

$$\Omega(x) < \inf_{\substack{x \in D \\ u \geqslant 0}} f_u(x, u) < 0 \qquad \text{for} \quad x \in D. \tag{3.2}$$

Define the sequence $\{u_n(x)\}$ by

$$\begin{aligned} Lu_0 &= -M(x), \qquad x \in D, \\ Bu_0 &= 0, \qquad x \in \partial D, \end{aligned} \tag{3.3}$$

$$Lu_n + \Omega(x)u_n = -f(x, u_{n-1}) + \Omega(x)u_{n-1}, \qquad x \in D, \qquad n = 1, 2, 3, \ldots,$$
$$Bu_n = 0, \qquad x \in \partial D.$$

THEOREM 3.1. *Let $f(x, u)$ satisfy* H-1 *to* H-4. *Then $u_n(x) > 0$ on D for all $n \geqslant 0$.*

Proof. The proof is by induction. The Positivity Lemma immediately implies that $u_0(x) > 0$ on D. Assume $u_\nu(x) > 0$ on D for all $\nu \leqslant n - 1$. Then, (3.2) and H-4 imply

$$\begin{aligned} Lu_n + \Omega u_n &= -f(x, u_{n-1}) + \Omega u_{n-1} \leqslant -f(x, u_{n-1}) + f_u(x, u_{n-1})u_{n-1} \\ &= u_{n-1}^2 \frac{d}{du}\left[\frac{f(x, u)}{u}\right]_{u=u_{n-1}} < 0, \qquad x \in D, \\ Bu_n &= 0, \qquad x \in \partial D. \end{aligned}$$

Hence, it follows from the Positivity Lemma with $a_0(x)$ replaced by $a_0(x) - \Omega(x)$ that $u_n(x) > 0$ on D. Q.E.D.

That the quantity $-f(x, u) + f_u(x, u)\, u$ is negative also follows from the geometric considerations of the Introduction. For fixed x the tangent to the curve $y = f(x, u)$ at the point $(v, f(x, v))$ is given by

$$y = f_u(x, v)\, u + [f(x, v) - f_u(x, v)\, v].$$

Thus, the quantity $[f(x, v) - f_u(x, v)\, v]$ determines where the tangent line intersects the axis of ordinates (i.e., the $u = 0$ axis). Conditions H-2 and H-4 and the definition (2.2) imply that this quantity is positive; that is, the tangent line must always intersect the positive y axis.

THEOREM 3.2. *Let $f(x, u)$ satisfy* H-1 *to* H-4. *Then, the sequence $\{u_n(x)\}$ defined by* (3.3) *is monotone nonincreasing; that is,*

$$u_{n+1}(x) \leqslant u_n(x), \qquad x \in D, \qquad n = 0, 1, 2, \ldots.$$

Proof. The proof is by induction. Equations (3.3) imply

$$\begin{aligned} L(u_0 - u_1) + \Omega(u_0 - u_1) &= -(M - f(x, u_0)) \leqslant 0, \qquad x \in D \\ B(u_0 - u_1) &= 0, \qquad x \in \partial D. \end{aligned}$$

Hence, by the obvious modification of the Positivity Lemma we conclude that $u_0(x) - u_1(x) \geqslant 0$ on D. Now, assume that $u_{\nu-1}(x) - u_\nu(x) \geqslant 0$ on D for all $\nu \leqslant n$. Then, from Eqs. (3.3) we have

$$\begin{aligned} L(u_n - u_{n+1}) + \Omega(u_n - u_{n+1}) &= f(x, u_n) - f(x, u_{n-1}) + \Omega(u_n - u_{n-1}) \\ &= f_u(x, \tilde{u})(u_n - u_{n-1}) + \Omega(u_n - u_{n-1}) \\ &= -[f_u(x, \tilde{u}) - \Omega](u_{n-1} - u_n) \leqslant 0, \quad x \in D, \end{aligned}$$

where $u_n \leqslant \tilde{u} \leqslant u_{n-1}$ and we have obviously used the Mean Value Theorem and then Eq. (3.2). Since $B(u_n - u_{n+1}) = 0$ on ∂D, The Positivity Lemma implies $u_n(x) - u_{n+1}(x) \geqslant 0$ on D. Q.E.D.

The existence of a positive solution is now established by

THEOREM 3.3. *Let $f(x, u)$ satisfy* H-1 *to* H-4. *Then, the sequence $\{u_n(x)\}$ defined by* (3.3) *converges to a positive solution of* (1.1), (1.2).

Proof. The proof follows from the work of Simpson and Cohen [7] for a similar problem. Since all details are given there, we shall content ourselves with the following brief outline:

Having demonstrated in Theorems 3.1 and 3.2 that the sequence $\{u_n(x)\}$ is monotone nonincreasing and bounded from below, we may immediately conclude that there is a limit function, say

$$\lim_{n\to\infty} [u_n(x)] = w(x) \geqslant 0 \qquad \text{for} \quad x \in D.$$

Clearly, the functions Lu_n are uniformly bounded, and the usual Schauder type estimates from the theory of elliptic equations implies that the u_n are equicontinuous. Thus, the limit function w is continuous, the convergence of the u_n to w is uniform and also the convergence of Lu_n is uniform. Hence, the compactness results of Agmon, Douglas, and Nirenberg [8] now imply that w is a solution of (1.1), (1.2). Q.E.D.

In anticipation of the uniqueness theorem of the next section we now construct a sequence $\{v_n(x)\}$ of iterates which converge to a positive solution monotonically from below. Once uniqueness is established, then by using both sequences, we can "pinch" the unique positive solution $u(x)$ of (1.1), (1.2) by solutions of linear equations as follows:

$$\begin{aligned} 0 \leqslant v_1 \leqslant \cdots \leqslant v_n \leqslant v_{n+1} \leqslant \cdots \leqslant u(x) \\ \leqslant \cdots \leqslant u_{n+1} \leqslant u_n \leqslant \cdots \leqslant u_1 \leqslant u_0 . \end{aligned} \tag{3.6}$$

The sequence $\{v_n(x)\}$ is defined by

$$v_0(x) \equiv 0$$

$$\begin{aligned} Lv_n + \Omega(x)v_n &= -f(x, v_{n-1}) + \Omega(x)v_{n-1}, \qquad x \in D, \qquad n = 1, 2, 3,..., \\ Bv_n &= 0, \qquad x \in \partial D. \end{aligned} \tag{3.7}$$

The proof that this procedure defines a monotone nondecreasing sequence of nonnegative functions is exactly like the proofs of Theorems 3.1, and 3.2 so we shall omit it. We show only how to establish a uniform upper bound on the iterates, and then the proof that they converge to a positive solution follows exactly like the proof of Theorem 3.3.

Clearly, $u_0(x) - v_0(x) \geqslant 0$ on D. Now, (3.3) and (3.7) imply that

$$\begin{aligned} L(u_n - v_n) + \Omega(u_n - v_n) &= -f(x, u_{n-1}) + f(x, v_{n-1}) + \Omega(u_{n-1} - v_{n-1}) \\ &= -[f_u(x, \tilde{u}) - \Omega](u_{n-1} - v_{n-1}), \end{aligned}$$

where we have obviously used the Mean Value Theorem. Hence, a straight forward induction argument allows us to prove that $u_n(x) - v_n(x) \geqslant 0$ on D, from which we conclude that for all $n \geqslant 1$ the $v_n(x)$ are uniformly bounded above by $\max_{x \in D} [u_0(x)]$.

4. Uniqueness of Positive Solutions

We shall need the

Lemma 4.1. *The sequence $\{u_n(x)\}$ defined by* (3.3) *converges to the maximal positive solution $\bar{u}(x)$ of* (1.1), (1.2); *that is, $\bar{u}(x) \geqslant u(x)$ on D for any positive solution $u(x)$.*

Proof. Assume $u(x)$ is any positive solution. Then, $u(x)$ satisfies

$$\begin{aligned} Lu &= -f(x, u), \qquad x \in D, \\ Bu &= 0, \qquad x \in \partial D. \end{aligned} \tag{4.1}$$

Equations (3.3) and (4.1) imply that

$$\begin{aligned} L(u_0 - u) &= -(M - f(x, u)) \leqslant 0, \qquad x \in D, \\ B(u_0 - u) &= 0, \qquad x \in D. \end{aligned}$$

The Positivity Lemma immediately implies that $u_0(x) - u(x) \geqslant 0$ on D. We now proceed by induction. Assume $u_\nu(x) - u(x) \geqslant 0$ on D for all $\nu \leqslant n - 1$.

Then,

$$L(u_n - u) = \Omega(u_{n-1} - u_n) - f(x, u_{n-1}) + f(x, u)$$
$$= -\Omega(u_n - u + u - u_{n-1}) - f_u(x, \tilde{u})(u_{n-1} - u),$$

where we have used the Mean Value Theorem and $u \leqslant \tilde{u} \leqslant u_{n-1}$. Hence,

$$L(u_n - u) + \Omega(u_n - u) = \Omega(u_{n-1} - u) - f_u(x, \tilde{u})(u_{n-1} - u)$$
$$= -[f_u(x, \tilde{u}) - \Omega](u_{n-1} - u) \leqslant 0, \qquad x \in D.$$
$$B(u_n - u) = 0, \qquad x \in D.$$

Therefore, from the Positivity Lemma we conclude that $u_n(x) - u(x) \geqslant 0$ on D; that is, $\{u_n(x)\}$ converges to the maximal positive solution. Q.E.D.

The main result of this section is the

THEOREM 4.2. *Let* $f(x, u)$ *satisfy* H-1 *to* H-5. *Then, positive solutions* (1.1), (1.2) *are unique.*

Proof. Let $\bar{u}(x)$ be the maximal positive solution, and suppose some other positive solution $v(x)$ exists. Then, $\bar{u}(x) \geqslant v(x)$ on D. Choose the *largest* number α_0 such that $v(x) \geqslant \alpha_0 \bar{u}(x)$ for all $x \in D$. Such an α_0 exists and satisfies $0 \leqslant \alpha_0 < 1$; this can be seen as follows: Let $A = \{\alpha \mid v(x) \geqslant \alpha \bar{u}(x)$ for all $x \in D\}$. A is nonempty since it obviously contains $\alpha = 0$, and clearly $\alpha \in A$ implies $0 \leqslant \alpha < 1$ since $\alpha \geqslant 1$ would contradict the fact that $\bar{u}(x)$ is the maximal positive solution. Thus, we have $\alpha_0 = \sup_\alpha A$.

Now, recalling property H-5, define

$$D_M = \{x \mid 0 < v(x) < b\}, \qquad D_m = \{x \mid b \leqslant v(x) \leqslant c\}.$$

For $0 \leqslant \alpha_0 < 1$ condition H-5 implies that

$$f[x, \alpha_0 \bar{u}(x)] > \alpha_0 \bar{u}(x) \frac{f[x, \bar{u}(x)]}{\bar{u}(x)} = \alpha_0 f[x, \bar{u}(x)]$$

for all $x \in \bar{D}$ such that $\bar{u}(x) > 0$. Hence, $f[x, \alpha_0 \bar{u}(x)] - \alpha_0 f[x, \bar{u}(x)] > 0$ for all $x \in \bar{D}$ [and also if $\bar{u}(x) = 0$]. In fact, by the continuity of

$$f(x, \alpha_0 \bar{u}) - \alpha_0 f(x, \bar{u})$$

and the boundedness of $f(x, \bar{u})$ there exists an $\epsilon_1 > 0$ such that

$$f[x, \alpha_0 \bar{u}(x)] - \alpha_0 f[x, \bar{u}(x)] \geqslant \epsilon_1 f[x, \bar{u}(x)]$$

for all $x \in \bar{D}$. Thus, for $x \in D_M$

$$\begin{aligned} -Lv &= f(x, v) \geqslant f(x, \alpha_0 \bar{u}) \\ &\geqslant (\alpha_0 + \epsilon_1) f(x, \bar{u}) = -(\alpha_0 + \epsilon_1) L\bar{u}, \end{aligned}$$

while for $x \in D_m$, the fact that $f(x, u)$ is a decreasing function of u implies

$$-Lv = f(x, v) \geqslant f(x, \bar{u}) = -[\alpha_0 + (1 - \alpha_0)] L\bar{u}.$$

Setting $\epsilon = \min[\epsilon_1, 1 - \alpha_0]$, we therefore have

$$Lv \leqslant (\alpha_0 + \epsilon) L\bar{u}, \qquad x \in D.$$

Hence,

$$\begin{aligned} L(v - (\alpha_0 + \epsilon)\bar{u}) &\leqslant 0, \qquad x \in D, \\ B(v - (\alpha_0 + \epsilon)\bar{u}) &= 0, \qquad x \in \partial D. \end{aligned}$$

Therefore, from the Positivity Lemma we conclude that $v(x) \geqslant (\alpha_0 + \epsilon)\bar{u}(x)$ on D which contradicts the fact that α_0 is the largest number such that $v(x) \geqslant \alpha_0 \bar{u}(x)$. Q.E.D.

We would like to point out how critical the geometry of the nonlinearity is for uniqueness. In the pertinent range $0 < u \leqslant c$ the condition H-4 implies that our nonlinearity $f(x, u)$ possesses the property that when graphed as a function of u for fixed x any straight line from the origin to the function lies below the graph of the function. It is easy to construct nonlinearities which violate this condition and for which the problem (1.1), (1.2) possesses more than one distinct positive solution on D (see T. W. Laetsch [5] for a more penetrating discussion).

All our results have been given for the general non-self-adjoint operator L. In the case that L is self-adjoint a particularly simple proof exists for Theorem 4.2. This consists of using the generalized Green's identity to write

$$\int_D (\bar{u}Lv - vL\bar{u})\, dx = 0,$$

where the zero on the right comes from the fact that the boundary conditions imply that the integral over ∂D vanishes. Now, if we take $\bar{u}(x)$ to be the maximal positive solution and $v(x)$ to be some other positive solution, we can write (using H-4)

$$0 = \int_D (\bar{u}Lv - vL\bar{u}) = \int_D \bar{u}v \left[\frac{-f(x, v)}{v} + \frac{f(x, \bar{u})}{\bar{u}}\right] < 0,$$

which is a contradiction. Hence $\bar{u}(x) \equiv v(x)$, and our proof is concluded for the self-adjoint case.

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