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A Numerical Test for the Existence and Uniqueness of Solution of Free Boundary Problems

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Abstract. The aim of this work is to introduce a numerical test for the existence and uniqueness of solution of free boundary problems governed by an ordinary differential equation. The main result is given by a theorem relating the existence and uniqueness question to the number of real zeros of a function implicitly defined within the formulation of the iterative transformation method. As a consequence, we can investigate the existence and uniqueness of solution by studying the behaviour of that function. Within such a context the numerical test is illustrated by two examples.

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1. Introduction.

We consider the numerical solution of the free boundary value problem (BVP)

$$
\begin{aligned}
&\frac{d^2u}{dx^2} = f\left(x, u, \frac{du}{dx}\right) \quad ; \quad x \in (0, s) \\
&g\left(u(0), \frac{du}{dx}(0)\right) = \alpha \quad ; \quad u(s) = j(s) \quad ; \quad \frac{du}{dx}(s) = \ell(s)
\end{aligned}
\tag{1.1}
$$

where $f(\cdot,\cdot,\cdot), g(\cdot,\cdot), j(\cdot)$ and $\ell(\cdot)$ satisfy appropriate smoothness conditions, α is a given constant and s represents the free boundary. The two conditions at $x = s$ are needed because s is unknown. By a solution of (1.1) we mean a pair (s, u), $s \in (0, \infty)$ and $u \in C^2(0, s)$, that verifies (1.1).

Free BVPs belonging to (1.1) arise in fields of current interest in biology, chemistry, engineering or mechanics [2–3, 5, 7, 9–10, 18–19]. Moreover, free BVPs of the form (1.1) are obtained from moving BVPs governed by partial differential equations via a similarity transformation [1 pp. 101–110].

Before considering the application of any numerical method a question naturally arises: Is the free BVP (1.1) well posed? Indeed, few results are known about the existence and uniqueness question. On this subject we can quote two papers [2–3] about particular problems governed by linear equations and a paper [23] on monotonicity properties, implying uniqueness, for a class of problems. Hence, any new idea for investigating that question is worth to be considered.

Here we prove a theorem relating the existence and uniqueness question to the number of real zeros of a "transformation function" defined within the formulation of the iterative transformation method (ITM). Then, as a numerical test for the existence and uniqueness of solution of (1.1) we propose the application of the ITM to look for the number of real zeros of that function. In this context a first application of the method was considered in [7].

The ITM discussed herein allows us to integrate numerically the class of free BVPs (1.1). However, the method in point can be extended to more general problems. For instance, the ITM was applied to a free BVP governed by a system of two first-order differential equations in [8]. The method in point allows us to transform a free BVP to a sequence of initial value problems. Such a transformation has also theoretical interest because it may represent an intermediate step to prove existence and uniqueness theorems (see [17 pp. 7-13]).

A first application of the ITM to a simple problem describing a biological model was given, on an intuitive basis, in [13]. Moreover, other applications arose in connection with: the length determination for a tubular chemical reactor [7], the shock front propagation in rate-type materials [8], the classical Stefan's problem [10] and the spreading of a viscous fluid under the influence of gravity [10]. A further application of the ITM to the numerical solution of BVPs on infinite intervals governed by a third-order ordinary differential equation was described in [12].

It was proved in [11] that the ITM is an extension of the non-ITM proposed in [13]. The ITM can also be applied to two-point BVPs and in this case it may be seen as an extension of the non-ITM discussed in [4]. However, the applicability of non-ITMs depends on the invariance properties of the governing differential equation and of the given boundary conditions. As a consequence, non-ITMs are considered as ad hoc methods (see [14, 18 pp. 35-36, 19 p. 137, 22 p. 218]). To the best of our knowledge the ITM is the first transformation method applicable to a general class of problems.

The remainder of the paper is organized as follows. In section 2 we define the ITM. In section 3 we provide a simple constructive proof of the main result that relates the existence and uniqueness of solution of free BVPs to the number of real zeros of the transformation function. Some guidelines on the definition of the transformation function and a discussion on its sensitivity analysis are developed in section 4. In section 5 we apply the method to two free BVPs describing, respectively, the length determination for a chemical catalytic converter [19] and the determination of the duration of motion in a simple dynamical context [19]. Our main concern is to verify numerically whether the considered problem has a unique solution. In this context the test indicates existence and uniqueness of solution for the first model and nonuniqueness for the second one. The last section is devoted to final remarks and conclusions. On the basis of the theorem proved in section 3, the proposed numerical test represents a possible way to investigate the existence and uniqueness of solution of free BVPs. Further evidences for this conclusion are given by the numerical experiments proposed in section 5 as well as by the study reported in [7].

2. The iterative transformation method.

By requiring the invariance of (1.1) with respect to a given transformation group we characterize a sub-class of problems (see [13] for the stretching and the spiral group and [6] for the translation group). As a consequence non-ITMs are applicable only to special classes of problems. To overcome this drawback we let all the arbitrary functions in (1.1) to depend also on a numerical parameter h, and in this way we introduce the problem

$$\begin{aligned} &\frac{d^2u}{dx^2} = F\left(x, u, \frac{du}{dx}, h\right) \\ &G\left(u(0), \frac{du}{dx}(0), h\right) = \alpha \quad ; \quad u(s) = J(s,h) \quad ; \quad \frac{du}{dx}(s) = L(s,h) \quad . \end{aligned} \tag{2.1}$$

This allows us to consider the extended stretching group

$$x^* = \lambda^\delta x \quad ; \quad s^* = \lambda^\delta s \quad ; \quad u^* = \lambda u \quad ; \quad h^* = \lambda^\sigma h \tag{2.2}$$

where δ and σ are constants different from zero and λ is the exponential of the group parameter. Our intention is to require the invariance of the governing differential equation and of the boundary conditions at $x = s$ in (2.1) with respect to (2.2) as well as that the following relations

$$G\left(u^*(0), \frac{du^*}{dx^*}(0), h^*\right) = \lambda\, G\left(u(0), \frac{du}{dx}(0), h\right) \quad , \tag{2.3}$$

and

$$\begin{aligned} &F\left(x, u, \frac{du}{dx}, 1\right) = f\left(x, u, \frac{du}{dx}\right) \\ &G\left(u(0), \frac{du}{dx}(0), 1\right) = g\left(u(0), \frac{du}{dx}(0)\right) \\ &J(s,1) = j(s) \\ &L(s,1) = \ell(s) \end{aligned} \tag{2.4}$$

are fulfilled. We impose (2.4) in order to recover (1.1) from (2.1) for $h = 1$. As far as the required invariance is concerned, a similarity analysis allows us to characterize the arbitrary functions in several equivalent ways; but the only functional form obeying the conditions (2.3) and (2.4) is the following

$$
\begin{aligned}
&F\left(x,u,\frac{du}{dx},h\right) = h^{(1-2\delta)/\sigma} f\left(h^{-\delta/\sigma}x, h^{-1/\sigma}u, h^{(\delta-1)/\sigma}\frac{du}{dx}\right)\\
&G\left(u(0),\frac{du}{dx}(0),h\right) = h^{1/\sigma} g\left(h^{-1/\sigma}u(0), h^{(\delta-1)/\sigma}\frac{du}{dx}(0)\right)\\
&J(s,h) = h^{1/\sigma} j(h^{-\delta/\sigma}s)\\
&L(s,h) = h^{(1-\delta)/\sigma}\ell(h^{-\delta/\sigma}s) \quad .
\end{aligned}
$$

Therefore, (2.1) reduces to the problem

$$
\begin{aligned}
&\frac{d^2u}{dx^2} = h^{(1-2\delta)/\sigma} f\left(h^{-\delta/\sigma}x, h^{-1/\sigma}u, h^{(\delta-1)/\sigma}\frac{du}{dx}\right)\\
&g\left(h^{-1/\sigma}u(0), h^{(\delta-1)/\sigma}\frac{du}{dx}(0)\right) = \alpha\ h^{-1/\sigma}\\
&u(s) = h^{1/\sigma} j(h^{-\delta/\sigma}s)\\
&\frac{du}{dx}(s) = h^{(1-\delta)/\sigma}\ell(h^{-\delta/\sigma}s) \quad .
\end{aligned}
\tag{2.5}
$$

Of course, a given problem belonging to (1.1) can always be embedded into (2.5) for every values of δ and σ different from zero. The requested invariance means that (2.2) transforms a problem of form (2.5) to a problem of the same form but with different values of $h, u(0), \frac{du}{dx}(0), s$ and α. In the following, without loss of generality, we assume $\alpha \neq 0$.

Let us consider the end value problem defined on $[0, s^*]$

$$
\begin{aligned}
&\frac{d^2u^*}{dx^{*2}} = h^{*(1-2\delta)/\sigma} f\left(h^{*-\delta/\sigma}x^*, h^{*-1/\sigma}u^*, h^{*(\delta-1)/\sigma}\frac{du^*}{dx^*}\right)\\
&u^*(s^*) = h^{*1/\sigma} j(h^{*-\delta/\sigma}s^*)\\
&\frac{du^*}{dx^*}(s^*) = h^{*(1-\delta)/\sigma}\ell(h^{*-\delta/\sigma}s^*) \quad ,
\end{aligned}
\tag{2.6}
$$

where δ, σ and s^* are considered to be fixed. If for every value of h^* the problem (2.6) is well posed, then $u^*(0)$ and $\frac{du^*}{dx^*}(0)$ are uniquely determined. Consequently, the application of invariance considerations allows us to obtain

$$
\lambda = \frac{h^{*1/\sigma}}{\alpha} g\left(h^{*-1/\sigma}u^*(0), h^{*(\delta-1)/\sigma}\frac{du^*}{dx^*}(0)\right)
\tag{2.7}
$$

and (for a positive value of λ)

$$
\begin{aligned}
&h = \lambda^{-\sigma}h^* \quad ; \quad u(0) = \lambda^{-1}u^*(0)\\
&\frac{du}{dx}(0) = \lambda^{\delta-1}\frac{du^*}{dx^*}(0) \quad ; \quad s = \lambda^{-\delta}s^* \quad .
\end{aligned}
\tag{2.8}
$$

A solution of (1.1) is determined when the value of $h = 1$ is obtained from (2.8). If s^*, δ and σ are fixed then λ is a function of h^* only, i.e., $\lambda = \lambda(h^*)$ where, in general, the functional form of $\lambda(\cdot)$ is not known. Thus, we are interested in the zeros of the "transformation function"

$$\Gamma(h^*) = [\lambda(h^*)]^{-\sigma} h^* - 1 \quad ; \quad \lambda > 0 \ . \tag{2.9}$$

This function is defined implicitly by the solution of the end value problem (2.6).

Along the lines of the analysis sketched above an iterative numerical method can be defined as follows:

- the original free BVP is embedded into (2.5) by fixing non-vanishing values of δ and σ;
- by setting a positive value of s^* and starting with suitable values of h_0^* and h_1^* a root-finding method is used to define a sequence h_i^*, for $i = 2, 3, \ldots,$. At each iteration $u^*(0)$ and $\frac{du^*}{dx^*}(0)$ are obtained by solving (2.6) numerically. The related sequences $s_i, \Gamma(h_i^*)$, for $i = 0, 1, 2, \ldots,$ are defined according to (2.7)–(2.9);
- suitable termination criteria have to be used to verify whether $\Gamma(h_i^*) \to 0$ as $i \to \infty$ (in that case also $s_i \to s$);
- having found an approximate value of s, a numerical approximation of $u(x)$ can be obtained by integrating (2.6) in the non-starred variables and with $h = 1$, inwards on $[0, s]$.

3. Existence and uniqueness

The main result of this paper can be stated as follows: for a given free BVP the existence and uniqueness question is reduced to finding the number of real zeros of the transformation function. This result is proved below.

Theorem. *Let us assume that s^*, δ and σ are fixed and that for every value of h^* the end value problem (2.6) is well posed on $[0, s^*]$. Then, the free BVP (1.1) has a unique solution if and only if the transformation function has a unique real zero; nonexistence (nonuniqueness) of the solution of (1.1) is equivalent to nonexistence of real zeros (existence of more than one real zero) of $\Gamma(\cdot)$.*

Proof by invariance considerations. We begin by proving that there exists a one-to-one and onto correspondence between the set of solutions of (1.1) and the set of real zeros of the transformation function. The thesis is an evident consequence of this result.

The mentioned correspondence can be defined as follows. For every values of δ and σ different from zero and $s^* > 0$, given a solution $(s, u(x))$ of (1.1) we can associate to it the real zero of $\Gamma(\cdot)$ defined by $h^* = (s^*/s)^{\sigma/\delta}$. The related value of $\lambda = (s^*/s)^{1/\delta}$, that is $\lambda = h^{*1/\sigma}$, allows us to verify by substitution in (2.9) that we have defined a real zero of the transformation function. Moreover, because of the invariance with respect to (2.2) the related solution of (2.6) is given by $u^*(x^*) = h^{*1/\sigma} u(h^{*\delta/\sigma} x)$ and is defined on $[0, s^*]$.

According to the definition of the transformation function, in general to each real zero h^* of $\Gamma(\cdot)$ there is related a solution $u^*(x^*)$, defined on $[0, s^*]$, of the end value problem (2.6). Now, the condition for $s^*, u^*(x^*), h^*$ to be transformed by (2.2) to $s, u(x), 1$ (where $u(x)$ is defined on $[0, s]$) is $\lambda = h^{*1/\sigma}$. Due to $\lambda = h^{*1/\sigma}$ we have

$u^*(0) = h^{*1/\sigma}u(0)$ and $\frac{du^*}{dx^*}(0) = h^{*(1-\delta)/\sigma}\frac{du}{dx}(0)$, so that the relation (2.7) implies that $u(x)$ verifies the boundary condition at zero in (1.1). Hence, to each real zero of $\Gamma(\cdot)$ we can associate a solution of (1.1). Again $\lambda = h^{*1/\sigma}$, so that $s = h^{*-\delta/\sigma}s^*$ and $u(x) = h^{*-1/\sigma}u^*(h^{*-\delta/\sigma}x^*)$.

It is easily seen that by means of the relations defined above we can fix both a right and left inverse of our correspondence. Therefore, the correspondence is one-to-one and onto. ∎

Before proceeding further some remarks are in order. First, by assuming $s^* - x^*$ as a new independent variable the end value problem (2.6) is transformed to an initial value problem defined on $[0, s^*]$. As far as initial value problems are concerned, the theory of well-posed problems is developed in detail in several classical books (see, for instance, [15, Chapters 2, 3 and 5]). In particular, the continuous dependence of the solution on parameters holds true provided suitable regularity conditions on $f(\cdot,\cdot,\cdot)$ are fulfilled. Second, if for every value of h^* we assume $\lambda(h^*) > 0$, then for $\delta \neq 0$ and each fixed value of h^* the scaling $[\lambda(h^*)]^{-\delta}x^* : [0, s^*] \to [0, s]$ is one-to-one and onto whereas the function of h^* defined by $[\lambda(h^*)]^{-\sigma}h^* : \mathbb{R} \to \mathbb{R}$ may not be one-to-one for $\sigma \neq 0$. Therefore, since $\Gamma(h^*) = [\lambda(h^*)]^{-\sigma}h^* - 1$, the transformation function may not be one-to-one. Third, by studying the behaviour of the transformation function it is possible to test the existence and uniqueness question.

4. The transformation function.

In this section we provide some guidelines for the definition of $\Gamma(\cdot)$. Let us define the function

$$\Xi(h^*, s^*, \delta, \sigma) = [\lambda(h^*, s^*, \delta, \sigma)]^{-\sigma}h^* - 1$$

by considering s^*, δ and σ as variables. Of course, for different values of these variables we obtain different transformation functions. In any case, the analysis proposed in the previous section does not depend upon the choice of the values of s^*, δ and σ. A sensitivity analysis for the dependence of $\Xi(\cdot,\cdot,\cdot,\cdot)$ with respect to s^*, δ and σ is not necessary because the ITM is defined for fixed values of these variables. As a consequence, once we have fixed the values of s^*, δ and σ it is unimportant if we use only approximations of these values. However, since s^* defines the range of integration for the end value problem (2.6) we propose to use $s^* = 0.5$ or $s^* = 1$. Actually, a value of $s^* \gg 1$ is not of interest here because of the global error accumulation for the numerical integration. Moreover, if the condition $s^* \in (0, \infty)$ is verified, then by the proof of the theorem we know in advance that every real zero of the transformation function belongs to $\mathbb{R}^+$ and therefore we can restrict the domain of $\Gamma(\cdot)$ to $\mathbb{R}^+$ whereupon its range will be reduced to $(-1, \infty)$. We remark that the values of δ and σ can always be chosen to consider only positive values of h^*.

On the other hand, the sensitivity of $\Gamma(\cdot)$ (and consequently of $\Xi(\cdot,\cdot,\cdot,\cdot)$) with respect to h^* is of particular interest. In fact, the numerical determination of the roots of $\Gamma(\cdot) = 0$ is a well-conditioned problem if and only if $|d\Gamma/dh^*|$ at the root is bigger than the machine rounding unit (a simple proof of this statement is possible under suitable regularity conditions on $\Gamma(\cdot)$). Therefore it is relevant to verify the sensitivity of $\Gamma(\cdot)$ at each zero. Of course, since $\Gamma(\cdot)$ is not given explicitly we cannot evaluate its sensitivity directly. Hence monitoring of the sensitivity will require an increase of the computational cost. A simple procedure is to apply as root-finding the secant method because in this case we compute at each iteration a finite difference approximation for the derivative of $\Gamma(\cdot)$. Caution has to be used because the finite difference approximation of derivatives is prone to rounding errors that could dominate the approximation.

Let us consider the definition of λ in (2.7), since $g\big(h^{*-1/\sigma}u^*(0), h^{*(\delta-1)/\sigma}\frac{du^*}{dx^*}(0)\big)$ is invariant with respect to the extended stretching group (2.2), $\lambda(h^*, s^*, \delta, \sigma)$ must have the following functional form

$$\lambda(h^*, s^*, \delta, \sigma) = h^{*1/\sigma}\lambda_0\big(h^{*-\delta/\sigma}s^*, \delta, \sigma\big)$$

so that

$$\Xi(h^*, s^*, \delta, \sigma) = [\lambda_0\big(h^{*-\delta/\sigma}s^*, \delta, \sigma\big)]^{-\sigma} - 1 \quad .$$

In other words, $\Gamma(\cdot)$ depends on $h^{*-\delta/\sigma}s^*$. This can be used when the zeros of the transformation function are very close to one endpoint of its domain. In particular, we can modify the value of δ or σ to define a transformation function with more amenable zeros (see the second example in the next section).

5. The numerical test and results.

In this section we test the ITM with respect to the existence and uniqueness question and obtain a numerical approximation of the free boundary value.

As a first example let us introduce the free BVP

$$\begin{aligned} &\frac{d^2u}{dx^2} = \frac{1}{u}\left(\frac{du}{dx}\right)^2 \quad ; \qquad x \in (0, s) \\ &u(0) = \alpha \;\; ; \quad u(s) = \beta \quad ; \quad \frac{du}{dx}(s) = \gamma \end{aligned} \tag{5.1}$$

that describes the diffusion of a gas in a chemical catalytic converter (see [19 pp. 79-80]). In that context u is related to the mole fraction of gas, x and s are, respectively, the coordinate along the converter and the unknown converter length. Moreover, $\alpha = -2+m_0, \beta = -2+\epsilon_m$ and $\gamma = -b_g$ where $0 < m_0 < 1, 0 < \epsilon_m < m_0$ and $b_g \gg 1$.

To apply the ITM we fix $\delta = -1$ and $\sigma = 2$ and consider the problem

$$\begin{aligned} &\frac{d^2u}{dx^2} = \frac{1}{u}\left(\frac{du}{dx}\right)^2 \\ &u(0) = \alpha \quad ; \quad u(s) = h^{1/2}\beta \quad ; \quad \frac{du}{dx}(s) = h\gamma \end{aligned} \tag{5.2}$$

that is partially invariant with respect to the extended stretching group (since $\alpha \neq 0$ the boundary condition $u(0) = \alpha$ is not invariant)

$$x^* = \lambda^{-1}x \quad ; \quad s^* = \lambda^{-1}s \quad ; \quad u^* = \lambda u \quad ; \quad h^* = \lambda^2 h \quad .$$

Due to the boundary condition $u(s) = h^{1/2}\beta$ we have to consider only positive values of h^*. For the physical parameters we take the following values:

$$\alpha = -1.75 \quad ; \quad \beta = -1.99 \quad ; \quad \gamma = -10 \quad , \tag{5.3}$$

so that $m_0 = 0.25, \epsilon_m = 0.01$ and $b_g = 10$.

TABLE 1. Problem (5.2)-(5.3).
Sample values of the transformation function for $s^* = 0.5$

h^*	$\Gamma(h^*)$
$1D+4$#	arithmetic fault, overflow
$1D+3$	$8.6D+34$
$1D+2$	$5.2D+21$
$1D+1$	$6.2D+6$
1	$1.2D+2$
$1D-1$	2.8
$1D-2$	0.278228150
$1D-3$	−0.093468297
$1D-4$	−0.186806707
$1D-6$	−0.222765036
$1D-9$	−0.226538043
$1D-12$	−0.226657057
$1D-15$	−0.226660820
$1D-18$	−0.226660939

Here and in the following the D notation indicates a double precision arithmetic.

Table 1 shows the behaviour of the transformation function. The numerical approximations indicate that $\Gamma(\cdot)$ tends to infinity as h^* goes to infinity and that it approaches, approximately, −0.226661 as h^* goes to zero. Therefore, at least one root of $\Gamma(h^*) = 0$ exists. A root-finding method was used and other numerical integrations, not listed in Table 1, were performed to verify that $\Gamma(h^*) = 0$ has only one root. The ITM was applied to obtain the iterations reported in Table 2.

TABLE 2. Numerical results for the problem (5.1)-(5.3). $s^* = 0.5$

i	h_i^*	$\Gamma(h_i^*)$	$\frac{du}{dx}(0)$	s
0	$1D-2$	0.278228150		
1	$1D-4$	−0.186806707		
...				
6	$2.616377D-3$	$1.3D-7$	−8.793970412	$2.5575262D-2$
7	$2.616374D-3$	$-9.3D-12$	−8.793969849	$2.5575251D-2$
8	$2.616374D-3$	$-1.4D-17$	−8.793969849	$2.5575251D-2$

As shown in Table 2 the last two iterated values for $\frac{du}{dx}(0)$ and for s agree up to nine decimal figures.

Problem (5.1) can be considered as a free boundary test problem, since we know its exact solution

$$s = \frac{\beta}{\gamma} \ln\left(\frac{\beta}{\alpha}\right) \quad ; \quad u(x) = \alpha \exp\left(\frac{\gamma}{\beta}x\right) . \tag{5.4}$$

We infer that (5.1) has a unique solution if and only if $\beta/\alpha > 1$ and $\beta/\gamma > 0$ or $1 > \beta/\alpha > 0$ and $\beta/\gamma < 0$; nonexistence of solution otherwise.

As far as the problem (5.1) is concerned, by integration it is possible to find

$$\lambda(h^*, s^*, \delta, \sigma) = h^{*1/\sigma}(\beta/\alpha)\exp(-(\gamma/\beta)h^{*-\delta/\sigma}s^*) \tag{5.5}$$

so that

$$\Xi(h^*, s^*, \delta, \sigma) = (\alpha/\beta)^\sigma \exp(\sigma(\gamma/\beta)h^{*-\delta/\sigma}s^*) - 1 . \tag{5.6}$$

From (5.4)–(5.6) we deduce that $\lambda < 0$ when $\alpha/\beta < 0$ (in this case the model has no physical meaning) and that all the obtained numerical results are correct.

As a second example we consider the free BVP, proposed in [19 p. 88],

$$\begin{aligned} &\frac{d^2u}{dx^2} = -u \exp(-u) \quad ; \quad x \in (0, s) \\ &u(0) = 0 \quad ; \quad u(s) = u_0 \quad ; \quad \frac{du}{dx}(s) = 0 \end{aligned} \tag{5.7}$$

where u is the coordinate of a unit mass moving, against the nonlinear force $-u \exp(-u)$, from the origin to a prescribed position (say $u = u_0$) along its path. We are interested in the initial velocity and in the duration of motion s, corresponding to a zero velocity at the final point. In the following we assume the final position to be $u_0 = 1$.

A similar problem was considered in [18 pp. 97–98], where the nonlinear force acting on the mass was assumed to be equal to $-1-u-\left(\frac{du}{dx}\right)^2$ (preliminary numerical results obtained with the ITM indicate that in this case the free BVP has a unique solution).

By using the transformation of variable $v(x) = u(x) + 1$, and fixing $\delta = 1/2$ and $\sigma = -2$, we get from (5.7) the problem

$$\begin{aligned} &\frac{d^2v}{dx^2} = (-vh^{1/2} + 1)\exp(-vh^{1/2} + 1) \\ &v(0) = 1 \quad ; \quad v(s) = (u_0 + 1)h^{-1/2} \quad ; \quad \frac{dv}{dx}(s) = 0 \end{aligned}$$

and the related stretching group

$$x^* = \lambda^{1/2}x \quad ; \quad s^* = \lambda^2 s \quad ; \quad v^* = \lambda v \quad ; \quad h^* = \lambda^{-2}h \quad .$$

The numerical results listed in Table 3 indicate nonuniqueness of solution for the problem (5.7). More zeros of the transformation function were found for $h^* \in (3.5D + 5, \infty)$; but with approximate values of $|d\Gamma/dh^*|$ at the zeros smaller than those reported in Table 3.

TABLE 3. Numerical results for the problem (5.7). $s^* = 0.5$

i	h_i^*	$\Gamma(h_i^*)$	$\frac{du}{dx}(0)$	s	$\frac{\Gamma(h_i^*)-\Gamma(h_{i-1}^*)}{h_i^*-h_{i-1}^*}$
0	$4D+2$	0.244988169			
1	$6D+2$	−0.11093691			
...					
7	$5.27D+2$	$-6D-16$	0.726967837	2.395989187	$-1.657279D-3$
0	$8D+3$	−0.149377948			
1	$1D+4$	0.2518297			
...					
5	$8.75D+3$	$-5.5D-15$	−0.726967837	4.835815681	$2.00893D-4$
0	$1.2D+5$	0.51368136			
1	$1.5D+5$	−0.282560928			
...					
7	$1.37D+5$	$-3.7D-15$	0.726967838	9.627794059	$-2.5466D-5$
0	$3.0D+5$	−0.451298446			
1	$3.5D+5$	0.140939878			
...					
7	$3.39D+5$	$-7.9D-15$	−0.726967839	12.06762055	$3.6966D-5$

As far as the problem (5.7) is concerned, a different transformation function can be defined by setting the values $\delta = -1/2, \sigma = -2$ and again $s^* = 0.5$. The related numerical results are not reported here for brevity. However, in that case several zeros were found for $h^* \to 0$ and this is in agreement with the theoretical result of the previous section. Moreover, the values of s listed in Table 3 were obtained also for the second set of values of δ, σ and s^*.

It seems that the differential equation admits two periodic solutions verifying the initial conditions $u(0) = 0$ and $\frac{du}{dx}(0) = \pm\ 0.726967838$. Let us show here that these values of $\frac{du}{dx}(0)$ are in agreement with the exact values up to seven decimal places. In fact, the governing differential equation admits the integral of energy

$$E\left(u, \frac{du}{dx}\right) = \frac{1}{2}\left(\frac{du}{dx}\right)^2 - (u+1)\ \exp(-u)$$

where, of course, E is constant. The constant value of E can be found by calculating $E(u_0, 0)$ and by evaluating $E(0, \frac{du}{dx}(0))$ we can obtain the value of $\frac{du}{dx}(0)$. Finally, in the case $u_0 = 1$ we get

$$\frac{du}{dx}(0) = \pm\ 0.726967811\ .$$

To carry out the numerical integrations we implemented a code in FORTRAN on an IBM RISC System/6000 using the DIVPAG subroutine of the IMSL Math

Library [16]. The Jacobian matrix and a local error bound of $1D-12$ were supplied to the DIVPAG subroutine. All iterations were performed by a secant method and the termination criteria used in the calculations were given by

$$|\Gamma(h_i^*)| < TOL \quad \text{and} \quad |s_i - s_{i-1}| < TOL$$

where TOL was $1D-9$ (see [21 pp. 226-228]). As indicated in [20] the iterations were continued as long as the value of $|s_i - s_{i-1}|$ was strictly monotone decreasing.

6. Final remarks and conclusions.

We propose the ITM to provide numerical evidence for the existence and uniqueness of solution of free BVPs on the basis of the theorem proved in section 3. The leading point is to establish whether the introduced transformation function has only one real zero or not. From a numerical viewpoint, several computations may be necessary to understand and to characterize the behaviour of $\Gamma(\cdot)$. For the proposed numerical test the transformation function was calculated at test-points while at some points a root-finding method was used. In the process we tried to bracket the roots of $\Gamma(\cdot) = 0$. In this way, it was possible to obtain numerical results that are in agreement with the correct values.

By setting different values of δ, σ and s^* we get a different transformation function and consequently we must bracket its zeros once again. However, we may get some hints from the previous study by taking into account that $\Gamma(\cdot)$ depends on $h^{*-\delta/\sigma}s^*$ (see the second numerical example in the previous section).

In conclusion, the main results of the present investigation are the following:

1. the ITM has a theoretical basis;
2. within the definition of the method we obtain a numerical test for the existence and uniqueness of solution of free BVPs;
3. the method provides numerical results that are in good agreement with the correct values.

Note added at proof. Very recently we apprehended that the problem (5.7), as a consequence of its integral of energy, has countably infinite many solutions (see SIAM Rev. 39 (1997) 136-138).

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