International Journal of Pure and Applied Mathematics

Volume 14 No. 4 2004, 463-492

USING PARAMETER CONTINUATION BASED ON THE MULTIPLE SHOOTING METHOD FOR NUMERICAL RESEARCH OF NONLINEAR BOUNDARY VALUE PROBLEMS

S.I. Fadeev[1 §], V.V. Kogai[2]

[1,2]Sobolev Institute of Mathematics
Russian Academy of Sciences
4, Pr. Koptyuga, Novosibirsk 630090, RUSSIA
[1]e-mail: fadeev@math.nsc.ru
[2]e-mail: kogai@math.nsc.ru

Abstract: Mathematical modelling of many physical processes leads to numerical research of nonlinear boundary value problems for ordinary differential equations. A very important aspect of it is to investigate the dependence of solutions on the model's parameters. To this end we consider the parameter continuation method based on the multiple shooting method in combination with a parameterization of the boundary value problem. Owing to the parameterization, the solution of the problem may be found in dependence on a chosen parameter of the model, including cases when there is branching of solutions of turning type.

AMS Subject Classification: 65L10
Key Words: mathematical model, nonlinear boundary value problem, ordinary differential equations, dependence of solutions, parameter continuation method, parameterization of the boundary value problem

1. The Concept of Well Conditionality for Nonlinear Boundary Value Problems

Consider a nonlinear boundary value problem for a system of N ordinary differential equations with a scalar argument x in the form:

Received: May 10, 2004

§Correspondence author

$$\begin{aligned} &\frac{dy}{dx} = f(x,y), \qquad x \in [a,b], \\ &g(y(a), y(b)) = 0, \end{aligned} \tag{1}$$

where y, f and g are vectors with components y_i, f_i and g_i, $i = 1, 2, \ldots, N$, respectively. The vector functions $f(x,y)$ and $g(y(a), y(b))$ are assumed sufficiently smooth with respect to all of their arguments, therefore the boundary value problem (1) has a solution $y = y(x)$ differentiable both with respect to x and with respect to all parameters that enter into the definition of the vector functions $f(x,y)$ and $g(y(a), y(b))$.

We say that the nonlinear boundary value problem (1) is well-posed (well-conditioned), if the linear boundary value problem:

$$\begin{aligned} &\frac{du}{dx} = A(x)u + F(x), \qquad x \in [a,b], \\ &Su(a) + Tu(b) = \varphi \end{aligned} \tag{2}$$

corresponding to (1) is well-posed. Here A, S and T are the Jacobi matrices:

$$A(x) = f_y(x, y(x)), \quad S = g_\alpha(y(a), y(b)), \quad T = g_\beta(y(a), y(b)), \tag{3}$$

$y(x)$ is the solution of the boundary value problem (1), $F(x)$ and φ are arbitrary, $F(x) \in C[a,b]$, $\alpha = y(a)$, $\beta = y(b)$.

It is known [1] that the well-conditionality of the boundary value problem (2) is equivalent to the boundedness of the norms of the matrix Green functions $G(x,t)$ and $G_0(x)$ satisfying the conditions:

1. $\dfrac{dG}{dx} = A(x)G, \qquad x \neq t,$
2. $G(t+0,t) - G(t-0,t) = I,$
3. $SG(a,t) + TG(b,t) = 0,$

for the matrix Green function $G(x,t)$, and

1. $\dfrac{dG_0}{dx} = A(x)G_0,$
2. $SG_0(a) + TG_0(b) = I,$

for the matrix Green function $G_0(x)$; here I is the identity matrix. The conditions uniquely define $G(x,t)$ and $G_0(x)$ if

$$\det\Big[SY(a) + TY(b)\Big] \neq 0,$$

where $Y(x)$ is the fundamental matrix of the homogeneous system with matrix $A(x)$.

A corollary of the bounds on the norms of the Green matrix functions is a norm estimate for the solution $u = u(x)$ of the boundary value problem (2), which follows from its integral representation

$$u(x) = \int_a^b G(x,t)F(t)\,dt + G_0(x)\varphi.$$

If K is the constant in the norm estimate for the matrix Green functions whose value describes the well-posedness of our boundary value problem, that is,

$$\|G(x,t)\| \le K, \qquad \|G_0(x)\| \le K,$$

then the norm of the solution of the boundary value problem can be estimated:

$$\max_x \|u(x)\| \le K \cdot \Big(\|\varphi\| + (b-a)\max_t \|F(t)\| \Big). \tag{4}$$

On the other hand, an estimate of the form (4) may be used as another definition of the well-posedness of the boundary value problem [2].

It is important to stress that if condition (4) is satisfied, then not only (2) is well-posed, but also the perturbed boundary value problem [1]

$$\begin{aligned} &\frac{d\tilde{u}}{dx} = \tilde{A}(x)\tilde{u} + \tilde{F}(x), \qquad x \in [a,b], \\ &\tilde{S}\tilde{u}(a) + \tilde{T}\tilde{u}(b) = \tilde{\varphi}, \end{aligned} \tag{5}$$

is well-posed if the matrices $\tilde{A}(x)$, $\tilde{S}$ and $\tilde{T}$ are close to $A(x)$, S and T respectively, i.e., if their perturbation norms are sufficiently small. Furthermore, if the perturbation norms of the right hand sides $F(x)$ and φ are small, then the boundary value problem (5) has a solution which is close to a solution of (2). Namely, if the conditions:

$$\max_x \left\| \tilde{A}(x) - A(x) \right\| \le \varepsilon, \qquad \max_x \left\| \tilde{F}(x) - F(x) \right\| \le \varepsilon,$$

$$\left\| \tilde{S} - S \right\| \le \frac{\varepsilon}{2}, \qquad \left\| \tilde{T} - T \right\| \le \frac{\varepsilon}{2}, \qquad \left\| \tilde{\varphi} - \varphi \right\| \le \varepsilon,$$

where

$$\varepsilon < \frac{1}{(1+b-a)K},$$

are satisfied, then the estimates:

$$\max_x \|\tilde{u}(x)\| \le U = \frac{K}{1-\varepsilon K(1+b-a)}\left(\|\tilde{\varphi}\| + (b-a)\max_t \|\tilde{F}(t)\|\right),$$

$$\max_x \|\tilde{u}(x) - u(x)\| \le \varepsilon(1+b-a)K(1+U)$$

hold. Henceforth, using sufficiently small perturbation norms of the matrices $A(x)$, S and T, we assume that the norms of the matrix Green functions of the boundary value problems (2) and (5) are bounded by the same constant K.

The meaning of the definition of the well-posedness of the nonlinear boundary value problem (1) introduced above becomes clear in the proof of the Newton method (quasilinearization method), which gives an iterative way of solving the boundary value problem (1), [9]. If the initial approximation $y^{[0]}(x)$ is sufficiently close to $y(x)$, then at every iteration the vector function $y^{[k]}(x)$, $k = 1, 2, \ldots$, approximating $y(x)$ is determined as the solution of a linear boundary value problem with matrices differing very little from $A(x)$, S and T. Therefore we may think about the well-conditionality of the linear boundary value problems at the iterations of the Newton method, and consequently, about the well-conditionality of the nonlinear boundary value problem to the solution of which the iterations converge. Let us consider this in more detail.

Denote by Ω a neighbourhood of the solution $y = y(x)$ of the boundary value problem (1) such that the boundary value problem (5) with matrices:

$$\tilde{A}(x) = f_y(x, \tilde{y}(x)), \qquad \tilde{S} = g_\alpha(\tilde{y}(a), \tilde{y}(b)), \qquad \tilde{T} = g_\beta(\tilde{y}(a), \tilde{y}(b)),$$

is well-posed if $\tilde{y}(x)$ is an arbitrary continuously differentiable vector function in Ω. Assume that $y^{[0]}(x) \in \Omega$. Then according to the Newton method, we construct an infinite sequence of vector functions $y^{[k]}(x)$, $k = 1, 2, \ldots$, determined from the linear boundary value problems:

$$\begin{aligned} &\frac{dy^{[k+1]}}{dx} = A^{[k]}(x)y^{[k+1]} + F^{[k]}(x), \qquad x \in [a,b], \\ &S^{[k]}y^{[k+1]}(a) + T^{[k]}y^{[k+1]}(b) = \varphi^{[k]}, \qquad k = 0, 1, 2, \ldots. \end{aligned} \tag{6}$$

Here we use the following notation:

$$A^{[k]}(x) = f_y(x, y^{[k]}(x)), \qquad F^{[k]}(x) = f(x, y^{[k]}(x)) - A^{[k]}(x)y^{[k]}(x),$$

$$S^{[k]} = g_\alpha(y^{[k]}(a), y^{[k]}(b)), \qquad T^{[k]} = g_\beta(y^{[k]}(a), y^{[k]}(b)),$$

$$\varphi^{[k]} = S^{[k]}y^{[k]}(a) + T^{[k]}y^{[k]}(b) - g(y^{[k]}(a), y^{[k]}(b)).$$

By virtue of our choice of $y^{[0]}(x)$, the boundary value problem (6) is well-posed at $k = 0$, and its solution in terms of the matrix Green functions $G^{[0]}(x,t)$ and $G_0^{[0]}(x)$ have the form:

$$y^{[1]}(x) = \int_a^b G^{[0]}(x,t)F^{[0]}(t)\,dt + G_0^{[0]}(x)\varphi^{[0]}.$$

Then as in the boundary value problem (2),

$$\left\|G^{[0]}(x,t)\right\| \le K, \qquad \left\|G_0^{[0]}(x)\right\| \le K.$$

Similar assertions hold for all other terms of the infinite sequence $y^{[k]}(x)$ if they belong to the region Ω.

Let us show that if $y^{[n]}(x) \in \Omega$, then $y^{[n+1]}(x) \in \Omega$ too. Indeed, let $y^{[n+1]}(x)$ be the solution of the boundary value problem (6) at $k = n$, and let $y(x)$ be the solution of the boundary value problem (1). Consider the difference $w(x) = y(x) - y^{[n+1]}(x)$. It is easy to see that we may assume that $w(x)$ is the solution of the boundary value problem:

$$\begin{aligned} &\frac{dw}{dx} = A^{[n]}(x)w + \tilde{F}(x), \qquad x \in [a,b], \\ &S^{[n]}w(a) + T^{[n]}w(b) = \tilde{\varphi}, \end{aligned} \tag{7}$$

where

$$\tilde{F}(x) = A^{[n]}(x)\Big(y^{[n]}(x) - y(x)\Big) + f\Big(x, y(x)\Big) - f\Big(x, y^{[n]}(x)\Big),$$

$$\begin{aligned} \tilde{\varphi} = {} & S^{[n]}\Big(y^{[n]}(a) - y(a)\Big) + T^{[n]}\Big(y^{[n]}(b) - y(b)\Big) \\ & + g\Big(y^{[n]}(a), y^{[n]}(b)\Big) - g\Big(y(a), y(b)\Big). \end{aligned}$$

Denoting by $G^{[n]}(x,t)$ and $G_0^{[n]}(x)$ the matrix Green functions of the boundary value problem (7), we represent its solution in the form:

$$w(x) = \int_a^b G^{[n]}(x,t)\tilde{F}(t)\,dt + G_0^{[n]}(x)\tilde{\varphi}.$$

By assumption $y^{[n]}(x) \in \Omega$, therefore

$$\left\| G^{[n]}(x,t) \right\| \le K, \qquad \left\| G_0^{[n]}(x) \right\| \le K.$$

Thus the estimate

$$\max_x \|w(x)\| \le K \cdot \left(\|\tilde{\varphi}\| + (b-a) \max_t \|\tilde{F}(t)\| \right)$$

holds. Then we use inequalities fulfilled by twice continuously differentiable vector functions, including the vector functions $f(x,y)$ and $g(y(a),y(b))$. In this case, there exist constants M and L such that

$$\max_x \|\tilde{F}(x)\|$$

$$= \max_x \left\| f(x,y(x)) - f(x,y^{[n]}(x)) - f_y(x,y^{[n]}(x))(y(x) - y^{[n]}(x)) \right\|$$

$$\le M \max_t \|y(t) - y^{[n]}(t)\|^2,$$

$$\|\tilde{\varphi}\| = \left\| g\Big(y(a),y(b)\Big) - g\Big(y^{[n]}(a),y^{[n]}(b)\Big) \right.$$

$$-g_\alpha\Big(y^{[n]}(a),y^{[n]}(b)\Big)\Big(y(a) - y^{[n]}(a)\Big)$$

$$\left. -g_\beta\Big(y^{[n]}(a),y^{[n]}(b)\Big) \cdot \Big(y(b) - y^{[n]}(b)\Big) \right\| \le L \max_t \left\| y(t) - y^{[n]}(t) \right\|^2.$$

This results to:

$$\max_x \|w(x)\| \le K \cdot (L + (b-a)M) \max_t \|y(t) - y^{[n]}(t)\|^2.$$

Thus if

$$K \cdot (L + (b-a)M) \max_t \|y(t) - y^{[n]}(t)\| < 1,$$

then

$$\max_x \|y(x) - y^{[n+1]}(x)\| \le \max_t \|y(t) - y^{[n]}(t)\|,$$

i.e., $y^{[n+1]}(x) \in \Omega$.

If the vector function $y^{[0]}(x)$ is so close to the solution of the boundary value problem (1) that

$$K \cdot (L + (b-a)M) \cdot \max_t \|y(t) - y^{[0]}(t)\| < 1, \tag{8}$$

then the following inequalities hold:

$$\max_x \|y(x) - y^{[1]}(x)\| \le K(L + (b-a)M) \max_t \|y(t) - y^{[0]}(t)\|^2$$

$$\le \max_t \|y(t) - y^{[0]}(t)\|,$$

$$\max_x \|y(x) - y^{[2]}(x))\| \le K \cdot (L + (b-a)M) \max_t \|y(t) - y^{[1]}(t)\|^2$$

$$\le K \cdot (L + (b-a)M) \max_t \|y(t) - y^{[0]}(t)\|^2 \le \max_t \|y(t) - y^{[0]}(t)\|,$$

and so on. Thus all the terms of the infinite sequence of vector functions $y^{[k]}(x)$, $k = 0, 1, 2, \ldots$, belong to the neighbourhood Ω. In other words, the boundary value problems (6) determining $y^{[k]}(x)$, $k = 1, 2, \ldots$, are well-posed by virtue of our choice of the initial approximation $y^{[0]}(x)$ sufficiently close to the solution of the boundary value problem (1). It is known that in this case $y^{[k]}(x)$ converge uniformly to the solution of the boundary value problem (1):

$$\lim_{k\to\infty} y^{[k]}(x) = y(x).$$

The matrices $A^{[k]}(x)$, $S^{[k]}$ and $T^{[k]}$ converge to $A(x)$, S and T respectively, i.e., they converge to the matrices: $f_y(x, y(x))$, $g_\alpha(y(a), y(b))$ and $g_\beta(y(a), y(b))$, and

$$\lim_{k\to\infty} G^{[k]}(x,t) = G(x,t), \qquad \lim_{k\to\infty} G_0^{[k]}(x) = G_0(x).$$

It follows that the solution of the boundary value problem (1) may be written in the form

$$y(x) = \int_a^b G(x,t)F(t)\,dt + G_0(x)\varphi,$$

where

$$F(x) = \lim_{k\to\infty} F^{[k]}(x) = f(x, y(x)) - A(x)y(x),$$

$$\varphi = \lim_{k\to\infty} \varphi^{[k]} = Sy(a) + Ty(b) - g(y(a), y(b)),$$

Therefore, it is natural to call the nonlinear boundary value problem (1) well-posed if the linear boundary value problem (2) is well-posed.

2. The Parameterized Boundary Value Problem

Suppose that Q is a parameter of our mathematical model, and we need to study how the solution of the boundary value problem (1) depends on Q. Accordingly, we rewrite (1) in the form:

$$\begin{aligned} &\frac{dy}{dx} = f(x, y, Q), \qquad x \in [a, b], \\ &g(y(a), y(b), Q) = 0, \qquad Q \in [Q_0, \bar{Q}]. \end{aligned} \tag{9}$$

Let us assume that the boundary value problems (1) and (9) coincide at $Q = Q_0$; thus, the boundary value problem (9) with solution $y(x, Q)$ is well-posed at $Q = Q_0$. This allows us to determine the derivative of the solution with respect to the parameter Q, i.e., we obtain a vector function $v(x) = y_Q(x, Q_0)$ which is the solution of the well-posed linear boundary value problem:

$$\begin{aligned} &\frac{dv}{dx} = A(x)v + R(x), \qquad x \in [a, b], \\ &Sv(a) + Tv(b) = \psi, \end{aligned} \tag{10}$$

where

$$A(x) = f_y\Big(x, y(x, Q_0), Q_0\Big), \qquad R(x) = f_Q\Big(x, y(x, Q_0), Q_0\Big),$$

$$S = g_\alpha\Big(y(a, Q_0), y(b, Q_0), Q_0\Big), \qquad T = g_\beta\Big(y(a, Q_0), y(b, Q_0), Q_0\Big),$$

$$\psi = -g_Q\Big(y(a, Q_0), y(b, Q_0), Q_0\Big).$$

Indeed, because $A(x)$, S and T are the matrices of the boundary value problem (2), the boundary value problem (10) is well-posed, and consequently, so is (9). Also we may assert that the boundary value problems (9) and (10) are well-posed at all values of Q in a neighbourhood of Q_0.

Recall that the solution of the boundary value problem (10) has an integral representation:

$$v(x) = \int_a^b G(x, t)R(t)\, dt + G_0(x)\psi. \tag{11}$$

The matrix Green functions $G(x, t)$ and $G_0(x)$ satisfy the conditions:

$$\|G(x, t)\| \le K, \qquad \|G_0(x)\| \le K.$$

Simultaneously with (9), consider the so-called parameterized boundary value problem with a parameter μ, which is defined as follows [5]:

$$\begin{aligned} &\frac{dy}{dx} = f(x, y, Q), \qquad x \in [a, b],\\ &\frac{dQ}{dx} = 0,\\ &g(y(a), y(b), Q) = 0,\\ &y_k(x_c, Q) = \mu, \quad x_c \in [a, b], \quad \mu \in [\mu_0, \bar{\mu}]. \end{aligned} \tag{12}$$

Here, unlike for the boundary value problem (9), we seek to determine the vector function $y(x, \mu)$ with a known value of the k-th component at $x = x_c$; therefore, in this case the parameter Q should also be determined, i.e., $Q = Q(\mu)$.

Note that the solution $y(x, Q_0)$ of the boundary value problem (9) at $Q = Q_0$ is the solution of the boundary value problem (12) at $\mu = \mu_0 = y_k(x_c, Q_0)$. Let us show that with a proper choice of the component index k and x_c, the boundary value problem (12) is possibly more well-posed than (9). In this case, we should find the vector function $y(x, Q_0)$ as the vector function $y(x, \mu_0)$ from the boundary value problem (12), rather than from (9). We keep solving (12) with the same choice of the component index in some neighbourhood of μ_0.

To this end, consider the linear boundary value problem for the derivatives $y_\mu(x, \mu_0)$ and $Q_\mu(\mu_0)$ of the solution of the boundary value problem (12) with respect to the parameter μ at $\mu = \mu_0$. Using the notation

$$z(x) = y_\mu(x, \mu_0), \qquad \theta = Q_\mu(\mu_0),$$

we may write the boundary value problem in the form:

$$\begin{aligned} &\frac{dz}{dx} = A(x)z + R(x)\theta, \qquad x \in [a, b],\\ &\frac{d\theta}{dx} = 0,\\ &Sz(a) + Tz(b) = \psi\theta, \qquad z_k(x_c) = 1, \qquad x_c \in [a, b], \end{aligned} \tag{13}$$

where $A(x)$, S and T are the same matrices, $R(x)$ and ψ are the same vectors as in the boundary value problem (10). Comparing the boundary value problems (10) and (13), we note that among the components $v_j(x)$, $j = 1, 2, \ldots, N$, of the vector function $v(x)$ there are such that

$$v_k(x_c) = \frac{dy_k}{dQ}(x_c, Q_0) = \mu_Q(Q_0) = \frac{1}{\theta} \neq 0.$$

It is easy to convince ourselves that in this case the solution of the boundary value problem (13) is the vector function

$$z(x) = \theta \cdot v(x) = \frac{v(x)}{v_k(x_c)},$$

or, taking into account the expression for $v(x)$ from (11),

$$z(x) = \int\limits_a^b \frac{G(x,t)}{v_k(x_c)} R(t)\,dt + \frac{G_0(x)}{v_k(x_c)}\psi.$$

This implies the estimate

$$\max_x \|z(x)\| \le K' \cdot \left(\|\psi\| + (b-a) \max_t \|R(t)\| \right), \tag{14}$$

where $K' = K/|v_k(x_c)|$. Then $K' < K$ if $|v_k(x_c)| > 1$. According to the definition of well-conditionality in the form of the estimate (4), it is natural to assume that the smaller is the constant K in that estimate, the more well-posed is the boundary value problem. In this sense, the boundary value problem (12) is more well-posed than the boundary value problem (9) if $|v_k(x_c)| > 1$.

Let $y(x, Q_0)$ be the solution of the boundary value problem (9) with components $y_j(x, Q_0)$, $j = 1, 2, \ldots, N$, at $Q = Q_0$, and let $v(x) = y_Q(x, Q_0)$ be the solution of the boundary value problem (10) for the derivatives of $y(x, Q)$ with respect to the parameter Q with components $v_j(x)$, $j = 1, 2, \ldots, N$ at $Q = Q_0$. Let us determine $v_k(x_c)$ by the conditions

$$|v_k(x_c)| = \max_{j,x} |v_j(x)|.$$

If $|v_k(x_c)| > 1$, then according to (14), the parameterized boundary value problem (12) with the parameter μ from a neighbourhood of $\mu_0 = y_k(x_c, Q_0)$ is more well-posed than the boundary value problem (9), and vice versa, if $|v_k(x_c)| < 1$, then the boundary value problem (9) with the parameter Q from a neighbourhood of Q_0 is more well-posed than the parameterized boundary value problem (12).

Note that by definition, the linear boundary value problem (13) for the derivatives of the solution with respect to the parameter μ is well-posed if the parameterized boundary value problem (12) is well-posed.

Parameterization is useful for solving many problems related to the numerical research of nonlinear boundary value problems. Let us mention one of them [5].

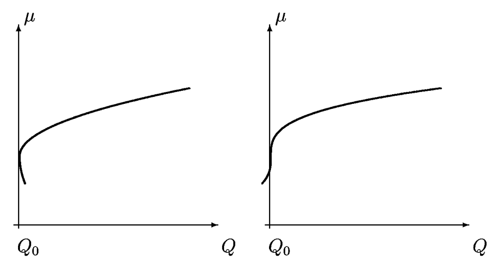

Figure 1:

Suppose that the nonlinear boundary value problem (9) has branching of solutions at $Q = Q_0$, i.e., Q_0 is an eigenvalue of the linear boundary value problem (10), thus

$$\det\Big[SY(a) + TY(b)\Big] = 0.$$

In the case of branching of solutions of turning type, the parameterized boundary value problem (11) with a properly chosen parameter μ allows us to determine numerically the dependence of the solution on μ in a neighbourhood of the branch point. The graphs of the dependence of Q on μ in a neighbourhood of Q_0 that may be obtained from solutions of the parameterized boundary value problem are represented in Figure 1. We will give a description of a regular use of parameterization in connection with the parameter continuation method.

3. The Multiple Shooting Method

A well-known method for solving the boundary value problem (1) numerically is the shooting method [16, 15, 10]. Consider the initial value problem for the system (1):

$$\begin{aligned} \frac{dy}{dx} &= f(x,y), \qquad x \in [a,b], \\ y\Big|_{x=a} &= p. \end{aligned} \tag{15}$$

Its solution is denoted by $y(x,p)$. Here p is a vector of initial values whose components should be found so that the boundary conditions (1) are satisfied, i.e.,

$$\Phi(p) \equiv g(p, y(b,p)) = 0. \tag{16}$$

Obviously, in this case the vector function $y(x,p)$ gives the solution of the boundary value problem (1), which we assume to exist. Thus the problem is reduced to solving the system of the nonlinear equations (16) with respect to the components of the vector p. Here the shooting correction is performed by the Newton method [16, 15, 10].

Let p^0 be the initial approximation of the solution in the Newton method for the system (16). Then for the correction Δp^0 refining p^0 we have a system of linear algebraic equations with matrix $\Phi_p(p^0)$:

$$\Phi_p(p^0)\Delta p^0 = -\Phi(p^0),$$

where

$$\Phi_p(p^0) = g_\alpha(p^0, y(b,p^0)) + g_\beta(p^0, y(b,p^0))y_p(b,p^0).$$

We then replace the initial approximation with the vector $p^1 = p^0 + \Delta p^0$, find the correction Δp^1 to it from the system of linear algebraic equations

$$\Phi_p(p^1)\Delta p^1 = -\Phi(p^1),$$

and repeat the process. The correction Δp^k to the approximation p^k is determined from the system of linear algebraic equations

$$\Phi_p(p^k)\Delta p^k = -\Phi(p^k), \qquad k = 1, 2, \dots,$$

where

$$\Phi_p(p^k) = g_\alpha(p^k, y(b,p^k)) + g_\beta(p^k, y(b,p^k))y_p(b,p^k), \tag{17}$$

therefore $p^{k+1} = p^k + \Delta p^k$. We then assume that the solutions of the initial value problems

$$\begin{aligned} &\frac{dy}{dx} = f(x,y), \qquad x \in [a,b],\\ &y\Big|_{x=a} = p^k, \qquad k = 0, 1, 2, \dots, \end{aligned} \tag{18}$$

are defined on $[a,b]$, and furthermore, that the initial approximation p^0 is sufficiently close to the solution of the system (16).

From (17) it follows that in order to perform iterations by the Newton method, we have to define the matrix of derivatives of the vector function $y(x,p^k)$ with respect to the components of the vector of initial values at $x = b$. Therefore, the initial value problem (18) is solved simultaneously with variation equations that determine the matrix function $V(x) = y_p(x,p^k)$:

$$\begin{aligned} &\frac{dV}{dx} = f_y(x, y(x,p^k))V, \qquad x \in [a,b],\\ &V\Big|_{x=a} = I. \end{aligned} \tag{19}$$

Note that the initial value problems (18) may be very 'stiff' although the boundary value problem (1) we are considering is well-posed. Applying the shooting method in this case is troublesome; we have here a problem analogous to the 'flattening' of the basis solutions of the homogeneous system of the equations (19), [1].

The multiple shooting method [15, 10] plays for the nonlinear boundary value problem (1) the same role as the Godunov orthogonal sweep method [13] does for a linear boundary value problem of type (2), allowing us to find the solution provided that the boundary value problem is well-posed. Divide the interval $[a, b]$ into m parts:

$$a = x_1 < x_2 < \ldots < x_m < x_{m+1} = b,$$

and on each subinterval $[x_i, x_{i+1}]$ consider the initial value problem

$$\begin{aligned} &\frac{dy}{dx} = f(x, y), \qquad x \in [x_i, x_{i+1}], \\ &y\Big|_{x = x_i} = p^{[i]}, \qquad i = 1, 2, \ldots, m, \end{aligned} \tag{20}$$

where $p^{[i]}$ is a vector of initial values. Construct simultaneously the solution $V(x, p^{[i]})$ is constructed of the initial value problem for the matrix equation

$$\begin{aligned} &\frac{dV}{dx} = f_y(x, y(x, p^{[i]}))V, \qquad x \in [x_i, x_{i+1}], \\ &V\Big|_{x = x_i} = I, \end{aligned} \tag{21}$$

where $y(x, p^{[i]})$ is the solution of the initial value problem (20). Obviously, the vector functions $y(x, p^{[i]})$, $i = 1, 2, \ldots, m$, together give the solution of the boundary value problem (1) if the conditions expressing the continuity of the solution at the mesh points of the interval $[a, b]$ and the boundary conditions

$$\begin{aligned} &\Phi^{[1]} = g(p^{[1]}, p^{[m+1]}) = 0, \\ &\Phi^{[2]} = y(x_2, p^{[1]}) - p^{[2]} = 0, \\ &\ldots \\ &\Phi^{[m+1]} = y(x_{m+1}, p^{[m]}) - p^{[m+1]} = 0 \end{aligned} \tag{22}$$

are satisfied. There results a system of nonlinear equations for the components of the vectors $p^{[1]}, p^{[2]}, \ldots, p^{[m+1]}$. Denote by p and Φ the vectors composed of the vectors $p^{[1]}$, $p^{[2]}, \ldots, p^{[m+1]}$ and $\Phi^{[1]}$, $\Phi^{[2]}, \ldots, \Phi^{[m+1]}$ respectively; this allows us to represent the system (22) in a vector form analogous to (16):

$$\Phi(p) = 0. \tag{23}$$

So unlike in the shooting method, in the multiple shooting method we find the components of the $m+1$ parts of the composed vector p (whence the method's name comes). Shooting is realized through the Newton method for the system (23) exactly as for the system (16). The Jacobi matrix used at the iterations is determined by the solutions of the initial value problem (21) and has the form

$$\Phi_p(p) =$$

$$\begin{bmatrix} g_\alpha(p^{[1]}, p^{[m+1]}) & & & & & & g_\beta(p^{[1]}, p^{[m+1]}) \\ V(x_2, p^{[1]}) & -I & & & & & \\ & V(x_3, p^{[2]}) & -I & & & & \\ & & \ddots & \ddots & & & \\ & & & \ddots & & -I & \\ & & & & V(x_{m+1}, p^{[m]}) & & -I \end{bmatrix}. \tag{24}$$

After the components of the vector p have been found, we may recover the solution of the problem (1) on the whole interval $[a, b]$ from the solutions of the initial value problems (20).

Note that the 'acceptable stiffness' of the initial value problem (20) is attained through a choice of the length of the integration interval $[x_i, x_{i+1}]$, and thus of the number of the mesh points on the interval $[a, b]$. Usually we impose the condition

$$D \cdot (x_{i+1} - x_i) \approx 1, \qquad \max_{x \in [x_i, x_{i+1}]} \left\| f_y(x, p^{[i]}) \right\| \leq D. \tag{25}$$

Furthermore, every time the homogeneous system (21) is to be integrated, we take the identity matrix (i.e., an orthogonal matrix) as the matrix of the initial values; because of our choice of the length of the interval $[x_i, x_{i+1}]$, this prevents the excessive flattening of basis solutions. In particular, when the multiple shooting method is used for solving a linear boundary value problem of type (2), we have in fact a variant of the Godunov orthogonal sweep method.

Let the boundary value problem (1) represent the boundary value problem (9) at $Q = Q_0$. The vector p determined by the system (23), i.e., the vector of mesh values of the solution of the boundary value problem (1), is the solution of the system

$$\Phi(p, Q) = 0 \tag{26}$$

at $Q = Q_0$. Let us apply the multiple shooting method to the linear boundary value problem (10) on $[a, b]$ for the derivative of the solution of the boundary value problem (9) with respect to the parameter Q at $Q = Q_0$. To determine the mesh values of the derivatives p_Q, we obtain a system of linear algebraic equations with matrix $\Phi_p(p, Q)$, which coincides with the matrix (24) at $Q = Q_0$:

$$\Phi_p(p, Q) p_Q = -\Phi_Q. \tag{27}$$

Indeed, denote by $v(x, p^{[i]})$ the solution of the initial value problem

$$\begin{aligned} &\frac{dv}{dx} = A(x)v + R(x), \qquad x \in [x_i, x_{i+1}], \\ &v\Big|_{x = x_i} = q^{[i]}, \qquad i = 1, 2, \ldots, m, \end{aligned} \tag{28}$$

Here

$$A(x) = f_y(x, y(x, p^{[i]}), Q_0), \qquad R(x) = f_Q(x, y(x, p^{[i]}), Q_0),$$

$q^{[i]}$ is the vector of initial values to be found from (31), and $y(x, p^{[i]})$ is the solution of the initial value problem (20). Note that $v(x, p^{[i]})$ may be written in the form

$$v(x, p^{[i]}) = V(x, p^{[i]}) q^{[i]} + v^0(x, p^{[i]}), \tag{29}$$

where the matrix function $V(x, p^{[i]})$ is determined from the conditions (21) and $v^0(x, p^{[i]})$ is the solution of the initial value problem

$$\begin{aligned} &\frac{dv^0}{dx} = A(x)v^0 + R(x), \qquad x \in [x_i, x_{i+1}], \\ &v^0\Big|_{x = x_i} = 0. \end{aligned} \tag{30}$$

The tuple of vector functions $v(x, p^{[i]})$, $i = 1, 2, \ldots, m$, represents the solution of the boundary value problem (10) under the following conditions, analogous to (22):

$$\begin{gathered} Sq^{[1]} + Tq^{[m+1]} - \psi = 0, \\ v(x_2, p^{[1]}) - q^{[2]} = 0, \\ \ldots \\ v(x_{m+1}, p^{[m]}) - q^{[m+1]} = 0, \end{gathered}$$

or, using (29),

$$\begin{aligned} &Sq^{[1]} + Tq^{[m+1]} = \psi, \\ &V(x_2, p^{[1]}) q^{[1]} - q^{[2]} = -v^0(x_2, p^{[1]}), \\ &\ldots\ldots\ldots\ldots\ldots \\ &V(x_{m+1}, p^{[m]}) q^{[m]} - q^{[m+1]} = -v^0(x_{m+1}, p^{[m]}), \end{aligned} \tag{31}$$

where

$$S = g_\alpha(p^{[1]}, p^{[m+1]}, Q_0), \qquad T = g_\beta(p^{[1]}, p^{[m+1]}, Q_0),$$

$$\psi = -g_Q(p^{[1]}, p^{[m+1]}, Q_0).$$

Hence if the tuple $p^{[1]}, \ldots, p^{[m+1]}$ is the solution of the system (22), then $q^{[1]}, \ldots, q^{[m+1]}$, satisfying the conditions (31), give the mesh values of the solution of the boundary value problem (10). Denoting by p_Q the vector composed of the vectors $q^{[1]}, q^{[2]}, \ldots, q^{[m+1]}$, and by Φ_Q the vector composed of the vectors

$$-\psi, v^0(x_2, p^{[1]}), \ldots, v^0(x_{m+1}, p^{[m]}),$$

we obtain a vector representation of the conditions (31) in the form of a system of linear algebraic equations (27).

4. Applying the Multiple Shooting Method to a Parameterized Boundary Value Problem

We shall verify that the multiple shooting method for a parameterized boundary value problem is realized in practice just as in the case of the boundary value problem (9). Again the problem reduces to a system of nonlinear equations defined by the solutions of a series of initial value problems for the mesh values of the solution of the parameterized boundary value problem (12). In what follows, we assume that $x_c = x_j$ in the boundary condition related to the introduction of the parameter μ, i.e.,

$$y_k(x_j, Q) = \mu,$$

where x_j is a mesh point of the interval $[a, b]$. In order to find our system of nonlinear equations, consider the series of initial value problems

$$\begin{aligned} &\frac{dy}{dx} = f(x, y, Q), \qquad x \in [x_i, x_{i+1}], \\ &y\Big|_{x = x_i} = p^{[i]}, \qquad i = 1, 2, \ldots, m. \end{aligned} \tag{32}$$

Denote the solution of (32) by a vector function $y(x, Q, p^{[i]})$, where $p^{[i]}$ is the vector of initial values. As for the system (22), we require that the tuple of vector functions $y(x, Q, p^{[i]})$ is the solution of the parameterized boundary value problem with the continuity condition at the mesh points of the interval $[a,b]$, and the boundary conditions

$$\begin{aligned}
&\Phi^{[1]} = g(p^{[1]}, p^{[m+1]}, Q) = 0,\\
&\Phi^{[2]} = y(x_2, Q, p^{[1]}) - p^{[2]} = 0,\\
&\dots\dots\dots\dots\dots\\
&\Phi^{[m+1]} = y(x_{m+1}, Q, p^{[m]}) - p^{[m+1]} = 0,\\
&\Phi^{[m+2]} = p_k^{[j]} - \mu = 0.
\end{aligned} \tag{33}$$

The system of nonlinear equations thus obtained determines the components of the vectors $p^{[1]}, p^{[2]}, \dots, p^{[m+1]}$ and the parameter Q in accordance with the parameter μ. Denote by $\tilde{p}$ the vector composed of the vectors $p^{[1]}$, $p^{[2]}, \dots, p^{[m+1]}$ and the parameter Q, and by $\tilde{\Phi}$ the vector composed of the vectors $\Phi^{[1]}$, $\Phi^{[2]}, \dots$, $\Phi^{[m+1]}$, $\Phi^{[m+2]}$. Then a vector representation of the system (33) takes the form

$$\tilde{\Phi}(\tilde{p}, \mu) = 0. \tag{34}$$

Let us find an expression for the Jacobi matrix $\tilde{\Phi}_{\tilde{p}}$ necessary for the determination of the components of the vector $\tilde{p}$ by the Newton method, as well as for the vector of derivatives $\tilde{p}_\mu$. To this end we apply the multiple shooting method to the linear boundary value problem (13), considering the series of initial value problems

$$\begin{aligned}
&\frac{dz}{dx} = A(x)z + R(x)\theta, \qquad x \in [x_i, x_{i+1}],\\
&z\Big|_{x = x_i} = q^{[i]}, \qquad i = 1, 2, \dots, m.
\end{aligned} \tag{35}$$

Here

$$A(x) = f_y(x, y(x, Q, p^{[i]}), Q), \qquad R(x) = f_Q(x, y(x, Q, p^{[i]}), Q),$$

$q^{[i]}$ is a vector of initial values, $y(x, Q, p^{[i]})$ is the solution of the initial value problem (32). Denote the solution of the initial value problem (35) by $z(x, Q, p^{[i]})$. If the vector $\tilde{p}$ with components $p^{[1]}, p^{[2]}, \dots, p^{[m+1]}$, Q is the solution of the system (34), then the conditions

$$\begin{aligned}
&Sq^{[1]} + Tq^{[m+1]} - \psi\theta = 0,\\
&z(x_2, Q, p^{[1]}) - q^{[2]} = 0,\\
&\dots\dots\dots\dots\dots\\
&z(x_{m+1}, Q, p^{[m]}) - q^{[m+1]} = 0,\\
&q_k^{[j]} - 1 = 0,
\end{aligned} \tag{36}$$

determine the vectors $q^{[1]}, q^{[2]}, \dots, q^{[m+1]}$ and θ — the components of the vector $\tilde{p}_\mu$ for which the functions $z(x, Q, p^{[i]})$, $i = 1, 2, \dots, m$, and θ represent the solution of the boundary value problem (13). Here

$$S = g_\alpha(p^{[1]}, p^{[m+1]}, Q), \qquad T = g_\beta(p^{[1]}, p^{[m+1]}, Q),$$

$$\psi = -g_Q(p^{[1]}, p^{[m+1]}, Q).$$

Now we use the fact that the solution of the boundary value problem (35) may be written in the form

$$z(x, Q, p^{[i]}) = V(x, Q, p^{[i]})q^{[i]} + z^0(x, Q, p^{[i]}), \tag{37}$$

where the matrix function $V(x, Q, p^{[i]})$ is the solution of the initial value problem (21) with matrix $A(x)$, and $z^0(x, Q, p^{[i]})$ is the solution of the boundary value problem for the non-homogeneous system of equations with the same matrix $A(x)$ and zero initial values:

$$\frac{dz^0}{dx} = A(x)z^0 + R(x)\theta, \qquad x \in [x_i, x_{i+1}],$$
$$z^0\Big|_{x = x_i} = 0.$$

The vector function $v^0(x, Q, p^{[i]})$ is the solution of the initial value problem (30), thus we obtain

$$z^0(x, Q, p^{[i]}) = \theta v^0(x, Q, p^{[i]}). \tag{38}$$

Using expressions (37) and (38), we reduce the system of linear algebraic equations (36) to the form

$$\begin{aligned}
&Sq^{[1]} + Tq^{[m+1]} - \psi\theta = 0,\\
&V(x_2, Q, p^{[1]})q^{[1]} - q^{[2]} + \theta v^0(x_2, Q, p^{[1]}) = 0,\\
&\dots\dots\dots\dots\dots\\
&V(x_{m+1}, Q, p^{[m]})q^{[m]} - q^{[m+1]} + \theta v^0(x_{m+1}, Q, p^{[m]}) = 0,\\
&q_k^{[j]} - 1 = 0,
\end{aligned}$$

or, using our notation for composed vectors,

$$\tilde{\Phi}_{\tilde{p}}(\tilde{p}, \mu)\tilde{p}_\mu = \ell, \tag{39}$$

where ℓ is the vector of right hand sides of the system of linear algebraic equations all of whose components are equal to zero except the last one which is equal to one. If we remember the expressions for the matrix Φ_p and the vector Φ_Q, then we can write the Jacobi matrix $\tilde{\Phi}_{\tilde{p}}$ of the system of nonlinear equations (34) in the form

$$\tilde{\Phi}_{\tilde{p}}(\tilde{p},\mu) = \left[\begin{array}{ccccc|c} & & \Phi_p & & & \Phi_Q \\ \hline 0 & \dots & 1 & \dots & 0 & 0 \end{array}\right].$$

Here

$$\Phi_p = \begin{bmatrix} S & & & & & T \\ V(x_2,Q,p^{[1]}) & -I & & & & \\ & V(x_3,Q,p^{[2]}) & -I & & & \\ & & \ddots & \ddots & & \\ & & & \ddots & -I & \\ & & & & V(x_{m+1},Q,p^{[m]}) & -I \end{bmatrix},$$

and Φ_Q is the column vector with components

$$-\psi, v^0(x_2,Q,p^{[1]}), v^0(x_3,Q,p^{[2]}), \dots, v^0(x_{m+1},Q,p^{[m]}).$$

The only non-zero element in the last row of the matrix $\tilde{\Phi}_{\tilde{p}}$ is in its $(k+(j-1)N)$-th column (recall that j is the index of the mesh point, and k is the index of the chosen component of the vector $p^{[j]}$).

The arguments we have presented allow us to formulate a uniform rule for solving numerically both the boundary value problem (9) and the boundary value problem (12) by the multiple shooting method. The rule reduces to defining nonlinear equations (26) or (34) respectively. Henceforth, we assume that μ is one of the components of the composed vector $\tilde{p}$, i.e., μ is either one of the components of the composed vector p or μ is the parameter Q. Consider a vector of unknowns X whose components are the components of the vector $\tilde{p}$ except μ. In accordance with these definitions of μ and X, the multiple shooting method results in a system of nonlinear equations

$$\Phi(X,\mu) = 0, \tag{40}$$

which coincides with the system (26) if $\mu = Q$, or with the system (34), where $p_k^{[j]}$ is omitted if $\mu = p_k^{[j]}$. Solving concurrently the series of initial value problems (20), (21) and (30) by the Newton method, we determine the vector Φ

and the matrix $[\Phi_p \quad \Phi_Q]$ and thus the Jacobi matrix Φ_X. Then Φ_X coincides with Φ_p if $\mu = Q$, i.e., in the matrix $[\Phi_p \quad \Phi_Q]$ the last column is deleted, or with the matrix $[\Phi_p \quad \Phi_Q]$, where the $(k + (j-1)N)$-th column corresponding to the component $p_k^{[j]}$ of the vector $\tilde{p}$ is deleted if $\mu = p_k^{[j]}$. With the iterations complete, the vector of derivatives X_μ is determined from the solution of the linear system of algebraic equations

$$\Phi_X(X(\mu), \mu)X_\mu = -\Phi_\mu(X(\mu), \mu), \tag{41}$$

where Φ_μ is the deleted column of the matrix $[\Phi_X \quad \Phi_Q]$. Thus we find the derivatives p_μ and Q_μ.

5. Parameterization and Parameter Continuation

Suppose that at $Q = Q_0$ we know both the solution of the boundary value problem (9) and its derivative with respect to the parameter Q. Then for Q_1 belonging to a sufficiently small neighbourhood of Q_0 we may choose an appropriate initial approximation $y^0(x, Q_1)$ of the solution of the boundary value problem (9) at $Q = Q_1$, for example, in the form

$$y^0(x, Q_1) = y(x, Q_0) + \Delta Q \cdot y_Q(x, Q_0), \tag{42}$$

where $\Delta Q = Q_1 - Q_0$ is the step of the parameter Q. Usually the size of the neighbourhood is not a priori known, thus while the solution $y(x, Q_1)$ is being determined, the parameter step may be improved. In particular, with the number of iterations in the Newton method restricted, if the required accuracy of approximations is not attained, the step is halved. This is one of the variants of step adaptation. Having obtained the solution $y(x, Q_1)$ and its derivative $y_Q(x, Q_1)$, we choose the initial approximation $y^0(x, Q_2)$, where Q_2 belongs to a sufficiently small neighbourhood of Q_1, and so on.

This method for solving numerically a boundary value problem depending on a parameter is known as the parameter continuation method or the homotopy method [6]. The parameter continuation for the parameterized boundary value problem (12) is realized in the same way, where vector functions $y(x, \mu)$ and $y_\mu(x, \mu)$ are used to form the initial approximation.

The capabilities of the parameter continuation method grow substantially if on each continuation step, after the solution and its derivatives with respect to the parameter have been obtained, we choose again a value of the parameter for continuing the solution one more step. We call the rule for making this choice, which we describe below, 'parameterization'. Further, in accordance with the results of parameterization, we choose an initial approximation either for the boundary value problem (9) or for the parameterized boundary value problem (12) using the derivatives of the solution with respect to the chosen parameter. Parameterization allows us to organize a regular computational process of finding the dependence of the solution of the boundary value problem (9) on the parameter Q. This includes the case when turning type branching of the solution occurs at some values of the parameter Q. We call the parameter value chosen for continuing the solution to the next step 'the current parameter'. The current parameter may be either the parameter μ of the parameterized boundary value problem, or the parameter Q. Below we denote the current parameter by μ, which should not cause any confusion.

Assume that on the interval of Q considered, the boundary value problem (9) with the solution $y(x, Q)$ may have singular points of turning type only. Denote by S_Q the graph of the vector function $y(x, Q)$ at an arbitrary value of Q in the $(N+1)$-dimensional Euclidean space (x, y). Varying the parameter Q continuously, we obtain in the space (x, y) a smooth surface Σ_Q swept by the space curves S_Q. As we have shown, the multiple shooting method reduces the problem of constructing the surface Σ_Q numerically to the system of nonlinear equations (26) for the mesh values of the vector function $y(x, Q)$, i.e., for the components of the composed vector $p(Q)$. Because Σ_Q is smooth, the system (26) defines a smooth space curve Γ_Q which is the graph of $p(Q)$ in the $(M+1)$-dimensional Euclidean space (p, Q), where $M = N(m+1)$. Then at the branch points of the solution of the boundary value problem (9) of turning type, the branching of solutions has the same type as for the system (26). Thus in a neighbourhood of a branch point, several solutions of the system (26) correspond to the same value of the parameter Q.

Because Γ_Q is smooth, the rank of the $(M \times (M+1))$-dimensional matrix $[\Phi_p \quad \Phi_Q]$ is equal, by the Implicit Function Theorem, to M in a neighbourhood of Γ_Q. In other words, taking into account the definitions of the vector X and the parameter μ of the system (40), for any point of Γ_Q there is a component μ of the vector $\tilde{p}$ equal to μ_0, and such that in a neighbourhood of μ_0

$$\det \Phi_X(X(\mu), \mu) \neq 0,$$

i.e., in the neighbourhood of μ_0 the system (40) has the solution $X(\mu)$ with its derivative $X_\mu(\mu)$.

Many different variants of continuation for a system of nonlinear equations of type (26) exist that determine a smooth space curve and deal with the possibility of branching of solutions of turning type appearing [6]. In this case, we suggest a variant of continuation concordant with the definition of a parameterized boundary value problem and using parameterization on each step for choosing the current parameter [7]. Note that the parameterized boundary value problem corresponds to the system of nonlinear equations (40) if the parameter μ does not coincide with Q.

Now we proceed to describe our parameterization procedure.

Suppose that at $\mu = \mu_0$ the solution $X(\mu_0)$ of the system (40) is known, as well as the vector of derivatives $X_\mu(\mu_0)$. Denote by $\tilde{\mu}_0$ the current parameter chosen among the components of the vector $X(\mu_0)$ and μ_0, i.e., among the components of the vector $\tilde{p}$. Denote the vector X corresponding to $\tilde{\mu}_0$ by $\tilde{X}$. Thus the solution of the system (40) at $\mu = \mu_0$ and the solution of the system

$$\Phi(\tilde{X}, \tilde{\mu}) = 0, \qquad \det \Phi_{\tilde{X}} \neq 0, \tag{43}$$

at $\tilde{\mu} = \tilde{\mu}_0$ represent the same vector $\tilde{p}$, whose components are the components $p_k^{[j]}$ of the vectors $p^{[j]}$ $k = 1, 2, \ldots, N$, $j = 1, 2, \ldots, m+1$, and Q. As above, we use $q_k^{[j]}$ and Q_μ to denote the components of the vector of derivatives $\tilde{p}_\mu$, in accordance with the notation for the components of the vector $\tilde{p}$. Obviously, the vector of derivatives $\tilde{p}_{\tilde{\mu}}$ with components $\tilde{q}_k^{[j]}$ and $Q_{\tilde{\mu}}$ is proportional to $\tilde{p}_\mu$:

$$\tilde{p}_{\tilde{\mu}} = \tilde{p}_\mu \cdot \left(\frac{d\tilde{\mu}}{d\mu}\right)^{-1}, \qquad \frac{d\tilde{\mu}}{d\mu} \neq 0. \tag{44}$$

In the parameterization procedure, a choice of the current parameter $\tilde{\mu}_0$ is realized as follows. By definition, the determination of the components of the vector of derivatives $X_\mu(\mu_0)$ means that the components of the vector $\tilde{p}_\mu$ become known. Put among them

$$\left| q_{k_*}^{[j_*]} \right| = \max_{k,j} \left| q_k^{[j]} \right|.$$

Three cases are possible here:

a) If $\left| q_{k_*}^{[j_*]} \right| > 1$ and $\left| q_{k_*}^{[j_*]} \right| > |Q_\mu|$, then the component $p_{k_*}^{[j_*]}$ of the vector $\tilde{p}$ is chosen as the current parameter $\tilde{\mu}$.

b) If $|Q_\mu| > 1$ and $|Q_\mu| > \left| q_{k_*}^{[j_*]} \right|$, then $\tilde{\mu} = Q$.

c) If $\left| q_{k_*}^{[j_*]} \right| \leq 1$ and $|Q_\mu| \leq 1$, then $\tilde{\mu} = \mu$, i.e., the current parameter μ, at which the solution of the system (40) is determined, remains the same.

Note that with this rule for choosing the current parameter, the inequality

$$\left| \det \tilde{\Phi}_{\tilde{X}} \right| \geq |\det \Phi_X| > 0$$

is satisfied [7]. Thus the solution of the system (40) at $\mu = \mu_0$ may indeed be considered as the solution of the system (43) at $\tilde{\mu} = \tilde{\mu}_0$.

The scheme we suggest for the parameter continuation of the solution of the system (26) by the current parameter, and thus also for the parameter continuation of the solution of the boundary value problem (9), has the following form. Suppose that at $Q = Q_0$ a solution of the boundary value problem (9) is known together with its derivative with respect to the parameter Q. It means that at $\mu = \mu_0 = Q_0$ the solution $X(\mu_0)$ of the system of nonlinear equations (40) and the vector of derivatives $X_\mu(\mu_0)$ are known. Using parameterization, we determine the current parameter $\tilde{\mu}$, the vector $\tilde{X}(\tilde{\mu}_0)$, and the vector of derivatives $\tilde{X}_{\tilde{\mu}}(\tilde{\mu}_0)$ through the normalization (44). After that, according to the parameter continuation, an initial approximation $\tilde{X}^0$ to the solution of the system (43) at $\tilde{\mu} = \tilde{\mu}_1$ is given in a form analogous to (42):

$$\tilde{X}^0 = \tilde{X}(\tilde{\mu}_0) + \Delta\mu \cdot \tilde{X}_{\tilde{\mu}}(\tilde{\mu}_0),$$

where $\Delta\mu = \tilde{\mu}_1 - \tilde{\mu}_0$. Having obtained the solution $\tilde{X}(\tilde{\mu}_1)$ of the system (43) at $\tilde{\mu} = \tilde{\mu}_1$ and the vector of derivatives $\tilde{X}_{\tilde{\mu}}(\tilde{\mu}_1)$ by the Newton method, we choose a new current parameter, and so on. Recall that the solution of the boundary value problem (9) can be recovered at all values of $x \in [a, b]$, together with its derivative with respect to the parameter Q, from the initial value problems (20), (21) and (30).

6. Applying the Parameter Continuation to Numerical Research of Periodic Solutions of Autonomous Systems

The parameter continuation method may be used for numerical research of periodic solutions of autonomous systems. Consider the problem of studying nonlinear oscillations described by an autonomous system of ordinary differential equations:

$$\frac{dy}{dt} = f(y, Q). \tag{45}$$

A periodic solution of the autonomous system (45), if it exists, satisfies the following condition:

$$y(t + T) = y(t),$$

where period T should be determined.

By adding boundary conditions to the system (45), the problem of finding periodic solutions of the autonomous system (45) may be reduced to the 'standard' statement of a nonlinear boundary value problem. The solution of the system (45) must be T-periodic by definition, thus it suffices to consider a boundary value problem on the interval $[0, T]$. The boundary conditions consist of the periodic conditions

$$y(0) = y(T), \tag{46}$$

and a transversality condition (phase condition), because the period is unknown.

The transversality condition may have various formulations; a choice of one, in general, depends on the particular system (45). Let us consider some formulations. In [3, 4] the following transversality conditions have been considered. Suppose that a sequence of solutions (45) corresponding to various values of the parameter Q of an autonomous system is known:

$$\{y^i(t), Q^i\}, \qquad i = 1, 2, \ldots, k-1.$$

Then for the determination of the next solution

$$\{y^k(t), Q^k\} = \{y(t), Q\},$$

the transversality condition is:

$$\left[y(0) - y^{k-1}\right]^* (y^{k-1}(0))' = 0$$

(this means that the derivative $(y^{k-1}(0))'$ and the vector $\left[y(0) - y^{k-1}\right]^*$ are orthogonal). It implies another transversality condition:

$$\int_0^T y^*(t)(y^{k-1}(t))' dt = 0.$$

We note here two other forms of transversality conditions that may be useful. Evidently, if $y(t)$ is a periodic solution of the autonomous system (45), the derivative $y'(t)$ is the periodic function too. Hence for each component of the vector function $y(t)$ there exists a point $c \in [0, T]$ such that

$$y_k'(c) = f_k(y(c), Q) = 0, \qquad 1 \leq k \leq N.$$

We may assume that $c = 0$, that is, the condition

$$f_k(y(0), Q) = 0 \tag{47}$$

may be considered a transversality condition, because the system (45) is autonomous.

Finally, consider a transversality condition which is not related to the choice of a component index. Multiply the equation (45) by $y(t)$

$$\left(y, \frac{dy}{dt}\right) = (y, f(y, Q)).$$

This leads to the equality

$$\frac{1}{2}\frac{d}{dt}\left\|y(t)\right\|^2 = \sum_{i=1}^{N} y_i(t) \cdot f_i(y(t), Q).$$

If $y(t)$ is a periodic solution of the autonomous system (45), then $\|y(t)\|^2$ is a periodic function too, thus, as in the previous case, a point c such that $\frac{d}{dt}\|y(t)\|^2 = 0$ exists and the equation

$$\sum_{i=1}^{N} y_i(0) \cdot f_i(y(0), Q) = 0$$

may be used as a transversality condition.

In order to reduce the problem to a standard form, make the substitution $t = Tx$, so that the solution $y(x)$ has period one. For example, add the transversality condition (47) to periodicity conditions (46). In this case we obtain a standard boundary value problem:

$$\begin{aligned}
&\frac{dy}{dx} = Tf(y, Q),\\
&\frac{dT}{dx} = 0,\\
&y(0) = y(1),\\
&f_k(y(0), Q) = 0, \qquad 1 \le k \le N.
\end{aligned} \tag{48}$$

If a periodic solution is found at $Q = Q_0$, it may be used as the initial solution of the boundary value problem (48) for the parameter continuation. For example, a stable periodic solution may be obtained by numerically integrating the system (45), [7].

7. Examples

Consider a nonlinear boundary value problem modelling stationary conditions of a catalytic reactor with a boiling layer [5].

$$\left.\begin{aligned} \frac{dy_1}{dx} &= y_2, \\ \frac{dy_2}{dx} &= s_0[(s_1+s_2)y_1 - s_2 y_3 - Q\varphi(y_1)y_4], \\ \frac{dy_3}{dx} &= s_2(y_1 - y_3), \\ \frac{dy_4}{dx} &= -s_3\varphi(y_1)y_4, \end{aligned}\right\} \quad 0 \le x \le 1, \quad Q \ge 0, \tag{49}$$

$$y_2(0) = y_3(0) = 0, \quad y_4(0) = 1, \quad y_2(1) = 0.$$

Here the functions $y_1(x)$, $y_3(x)$ and $y_4(x)$ describe, respectively, the dimensionless distributions of the temperatures of catalyzer and gas, and of concentration:

$$\varphi(y_1) = \left[s_5 + \exp\left(-\frac{y_1 + s_4}{1 + s_6(y_1 + s_4)}\right)\right]^{-1}.$$

The parameters of the problem are $s_1 = 8$, $s_2 = s_3 = 5$, $s_4 = -4$, $s_5 = 0,5$, $s_6 = 0,05$, $s_0 > 0$. This problem is characterized by the non-uniqueness of solutions. It is easy to verify that

$$Q = s_3 \frac{s_1\sigma + y_3(1)}{1 - y_4(1)}, \quad \sigma = \int_0^1 y_1(x)\,dx$$

follow from the boundary value problem (49). To visualize the non-uniqueness, we choose the graph of the dependence of Q on σ defined in the parameter continuation. In Figure 2 the graphs of the function $Q(\sigma)$ are represented for some values of s_0. Here the number of solutions of the boundary value problem (49) is equal to the number of intersections of the graph with the line Q=const. Note that for sufficiently large values of Q, only one solution exists.

For our second example, consider the following system — the Lorenz model [14]:

$$\begin{aligned} \frac{dx}{dt} &= -\sigma x + \sigma y, \\ \frac{dy}{dt} &= -xz + Qx - y, \\ \frac{dz}{dt} &= xy - bz, \end{aligned} \tag{50}$$

where σ, Q and b are parameters.

Changing the variable $t = Ts$ in the system (50), we obtain a nonlinear boundary value problem in the form:

$$
\begin{aligned}
&\frac{dx}{ds} = T \cdot (-\sigma x + \sigma y), \qquad s \in [0,1],\\
&\frac{dy}{ds} = T \cdot (-xz + Qx - y),\\
&\frac{dz}{ds} = T \cdot (xy - bz),\\
&\frac{dT}{ds} = 0,\\
&x(0) = x(1), \qquad y(0) = y(1), \qquad z(0) = z(1),\\
&-x(0)z(0) + Qx(0) - y(0) = 0.
\end{aligned}
$$

More than twenty branches of periodic solutions of the Lorenz model exist at $\sigma = 16$, $b = 4$ [8]. Some of them, obtained by the parameter continuation method, are shown in Figure 3.

8. Conclusion

Existing software packages that implement the parameter continuation method for nonlinear boundary value problems use various collocation methods, permitting one to formulate the problem approximately in the form of a system of nonlinear equations. Then in the continuation method, the possible appearance of branch points of turning type is dealt with.

In this paper we propose a method that has the same capabilities, but the system of nonlinear equations defined on the solutions of a series of initial value problems is the result of *an exact transformation* of the nonlinear boundary value problem. The correctness and efficiency of the proposed method is based on:

1. a regular parameterization of the problem during parameter continuation, with a specified rule for choosing the current parameter;

2. an application of the orthogonal differential sweep method at the iterations of the Newton method in the multiple shooting method for forming a linear system of algebraic equations;

3. taking advantage of the structure of the matrix while solving the linear algebraic system;

4. step adaptation depending on the current parameter and mesh adaptation along the x-variable during parameter continuation.

This method may also be used for numerical research of periodic solutions of autonomous systems.

References

[1] S.K. Godunov, *Ordinary Differential Equations with Constant Coefficients*, Volume **1**: *Boundary Value Problems*, Novosibirsk, Novosibirsk State University (1994), In Russian.

[2] S.K. Godunov, V.S. Ryabenki, *Difference Schemes*, Moscow, Nauka (1977), In Russian.

[3] E.J. Doedel, *Numerical Analysis and Control of Bifurcation Problems*, Montreal (1986).

[4] E.J. Doedel, J.P. Kernevez, *Auto: Software for Continuation and Bifurcation Problems in Ordinary Differential Equations*, Including the AUTO 86 User Manual, Pasadena, Calif. (1986).

[5] I.S. Fadeev, The program for numerical solving of nonlinear boundary value problems for systems of ordinary differential equations with parameters, *Trudi Instituta Matematiki, SB AS USSR — Computational Methods of Linear Algebra*, **17**, Novosibirsk (1990), 104-198, In Russian.

[6] S.I. Fadeev, S.A. Pokrovskaya, A.Yu. Berezin, I.A. Gainova, *Software Package STEP for Numerical Research of General Nonlinear Systems of Equations and Autonomous Systems*, Novosibirsk, Novosibirsk State University (1998), In Russian.

[7] M. Holodniok, A. Klic, M. Kubicek, M. Marek, *Analysis Methods for Nonlinear Dynamical Models*, Moscow, Mir (1991), In Russian.

[8] M. Holodniok, M. Kubicek, Derper — an algorithm for the continuation of periodic solutions in ordinary differential equations, *Journal of Computational Physics*, **55**, No. 2 (1984), 254-267.

[9] L.V. Kantorovich, G.P. Akilov, *Functional Analysis in the Norm Spaces*, Moscow (1959), In Russian.

[10] H.B. Keller, *Numerical Methods for Two-Point Boundary-Value Problems*, Ontario, London (1968), 184.

[11] V.V. Kogai, Using parameter continuation for numerical research of periodic solutions of autonomous systems of ordinary differential equations, *Vestnik, Quart. J. of Novosibirsk State University, Series: Mathematics, Mechanics and Informatics*, **2**, No. 1 (2002), 40-48, In Russian.

[12] V.V. Kogai, S.I. Fadeev, Use of parameter continuation on the basis of multple shooting method for numerical research of nonlinear boundary value problems, *Siberian Journal of Industrial Mathematics*, Novosibirsk, Institute of Mathematics of SB RAS, **4**, No. 1 (2001), 83-101, In Russian.

[13] S.V. Kuznetsov, The solving of the boundary value problems for ordinary differential equations, *Trudi Instituta Matematiki — Computational Methods of Linear Algebra*, SB AS USSR, Novosibirsk, **6** (1985), 85-110, In Russian.

[14] E.N. Lorenz, Deterministic nonperiodic flow, *Journal of Atmospheric Sciences*, **20**, No. 2 (1963), 130-141.

[15] G. Hall, J.M. Watt, Ed-s., *Modern Numerical Methods for Ordinary Differential Equations*, Clarendon Press, Oxford (1976).

[16] J.M. Ortega, W.C. Rheinboldt, *Iterative Solution of Nonlinear Equations in Several Variables*, N.Y., London (1970).

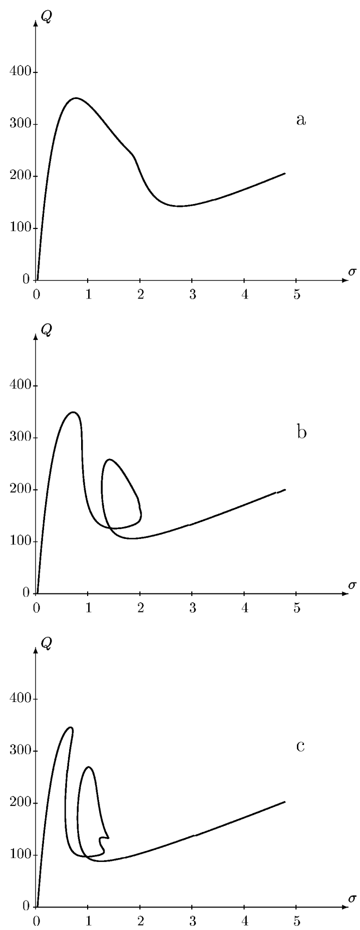

Figure 2: Graphs of the function $Q(\sigma)$: a) $s_0 = 1$, b) $s_0 = 5$, c) $s_0 = 20$

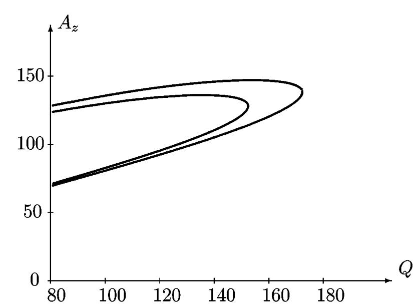

Figure 3: Dependence of the amplitude A_z of $z(t)$ on the parameter Q.