

## ADJOINT SYSTEM IN THE SHOOTING METHOD TO SOLVE BOUNDARY VALUE PROBLEMS

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### Abstract

The shooting method is used to solve a boundary value problem with separated and explicit constraints. To obtain approximations of an unknown initial values there are considered arguments based on the adjoint differential system attached to the given differential system. Finally the Newton-Kantorovich iterations are regained.

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*Key words*: shooting method, adjoint system.

## 1 Indroduction

The shooting method to solve a boundary value problem (BVP) is presented in many textbooks [1], [8], [5], [4]. In this note we consider the case of separated and explicit boundary conditions. For some variables the initial value is given and for the rest its are unknown. In essence the scope of the shooting method is to compute the unknown initial values in order to satisfy the ending conditions.

To use / implement the method two ingredients are necessary:

- A method / routine to integrate an initial value problem;
- A method / routine to solve an algebraic system. For a nonlinear algebraic system the Newton-Kantorovich method is widely used.

Practical aspects of implementing the shooting method are given in [6, 7].

In this note we point out a connection with an adjoint system attached to the differential system of the BVP. Trying to compute the unknown initial values using adjoint functions we regain the Newton-Kantorovich iterations.

The paper is organized as follows. After defining the BVP in Section 2, the shooting method is revisited in Section 3. In Section 4 the connection with adjoined system is detailed. Finally, in Section 5 numerical results for several examples are given.

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## 2 The boundary value problem with explicit boundary constraints

The considered BVP is defined by a system of ordinary differential equations

$$\dot{x}(t) = f(t, x(t)), \quad t \in [0, T], \quad (1)$$

and the boundary conditions

$$\begin{aligned} x_i(0) &= y_{0,i}, & i \in \mathcal{J}_0 \subset \{1, 2, \dots, n\}, & & |\mathcal{J}_0| &= m \\ x_j(T) &= y_{T,j}, & j \in \mathcal{J}_T \subset \{1, 2, \dots, n\}, & & |\mathcal{J}_T| &= n - m. \end{aligned} \quad (2)$$

where  $f : [0, T] \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ ,  $\mathcal{J}_0, \mathcal{J}_T, y_0 \in \mathbb{R}^m$ ,  $y_T \in \mathbb{R}^{n-m}$  are given. The function  $f(t, x)$  is twice continuously differentiable. By  $|\mathcal{J}_0|, |\mathcal{J}_T|$  we noted the number of elements of the corresponding sets. Let be  $\mathcal{J}_0^c = \{1, 2, \dots, n\} \setminus \mathcal{J}_0$ , the set of index for which the initial values are unknown.

We will use the matrices  $P_T \in M_{n-m, n}(\{0, 1\})$ ,  $P_0^c \in M_{n-m, n}(\{0, 1\})$  with the following definitions:

If  $\mathcal{J}_T = \{k_1, k_2, \dots, k_{n-m}\}$  with  $k_1 < k_2 < \dots < k_{n-m}$  then

$$(P_T)_{i,j} = \begin{cases} 1 & \text{if } j = k_i, \\ 0 & \text{otherwise} \end{cases} \quad \begin{matrix} i \in \{1, 2, \dots, n-m\} \\ j \in \{1, 2, \dots, n\} \end{matrix}$$

and  $P_0^c$  is defined analogously, corresponding to the set  $\mathcal{J}_0^c$ .

We suppose that the BVP has at least a solution.

For simplicity let be  $\mathcal{J}_0 = \{1, 2, \dots, m\}$  and  $\mathcal{J}_T = \{j_1, j_2, \dots, j_{n-m}\}$ . Then the boundary conditions are

$$\begin{aligned} x_i(0) &= y_{0,i}, & i \in \{1, 2, \dots, m\} \\ x_{j_k}(T) &= y_{T,k}, & k \in \{1, 2, \dots, n-m\} \end{aligned} .$$

Because  $\mathcal{J}_0^c = \{m+1, \dots, n\}$  it follows that  $P_0^c = [0_{n-m, m} \ I_{n-m}]$ .

## 3 Recall of the shooting method

We shall follow J. Singh's presentations [6, 7].

If the initial value of (1) is

$$x_0(c) = \begin{bmatrix} y_0 \\ c \end{bmatrix} \quad \Leftrightarrow \quad P_0^c x_0(c) = c, \quad (3)$$

with  $c \in \mathbb{R}^{n-m}$ , then the boundary conditions in  $T$  may be written as

$$F(c) = P_T x(T; x_0(c)) - y_T = \begin{pmatrix} x_{j_1}(T; x_0(c)) - y_{T,1} \\ \vdots \\ x_{j_{n-m}}(T; x_0(c)) - y_{T, n-m} \end{pmatrix} = 0. \quad (4)$$

(4) represents an algebraic system of  $n - m$  equations where the components of  $c = (c_1, \dots, c_{n-m})^T$  are the unknowns. The symbol  $^T$  marks the transpose of a matrix.

The Newton-Kantorovich methods may be used to solve this system. Then the following recurrence formula is applied:

$$c^{k+1} = c^k - (F'(c^k))^{-1}F(c^k), \quad k = 0, 1, 2, \dots \quad (5)$$

In order to compute  $F(c^k)$ , the initial value problem (1)-(3), with  $c = c^k$ , must be integrated. The computation of the matrix

$$F'(c) = P_T \frac{\partial x(T; x_0(c))}{\partial c} = \begin{pmatrix} \frac{\partial x_{j_1}(t; x_0(c))}{\partial c_1} & \dots & \frac{\partial x_{j_1}(t; x_0(c))}{\partial c_{n-m}} \\ \vdots & & \vdots \\ \frac{\partial x_{j_{n-m}}(t; x_0(c))}{\partial c_1} & \dots & \frac{\partial x_{j_{n-m}}(t; x_0(c))}{\partial c_{n-m}} \end{pmatrix}$$

is detailed below.

From

$$\begin{aligned} \frac{d}{dt} \frac{\partial}{\partial c_j} x_i(t; x_0(c)) &= \frac{\partial}{\partial c_j} \frac{d}{dt} x_i(t; x_0(c)) = \\ &= \frac{\partial}{\partial c_j} f_i(t, x(t; x_0(c))) = \sum_{k=1}^n \frac{\partial f_i(t, x(t; x_0(c)))}{\partial x_k} \frac{\partial x_k(t; x_0(c))}{\partial c_j} \end{aligned}$$

it results that

$$\begin{aligned} \frac{d}{dt} \underbrace{\begin{pmatrix} \frac{\partial x_1(t; x_0(c))}{\partial c_1} & \dots & \frac{\partial x_1(t; x_0(c))}{\partial c_{n-m}} \\ \vdots & & \vdots \\ \frac{\partial x_n(t; x_0(c))}{\partial c_1} & \dots & \frac{\partial x_n(t; x_0(c))}{\partial c_{n-m}} \end{pmatrix}}_{\frac{\partial x(t, x_0(c))}{\partial c}} &= \quad (6) \\ &= \underbrace{\begin{pmatrix} \frac{\partial f_1(t, x)}{\partial x_1} & \dots & \frac{\partial f_1(t, x)}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_n(t, x)}{\partial x_1} & \dots & \frac{\partial f_n(t, x)}{\partial x_n} \end{pmatrix}}_{f'(t, x(t; x_0(c)))} \underbrace{\begin{pmatrix} \frac{\partial x_1(t; x_0(c))}{\partial c_1} & \dots & \frac{\partial x_1(t; x_0(c))}{\partial c_{n-m}} \\ \vdots & & \vdots \\ \frac{\partial x_n(t; x_0(c))}{\partial c_1} & \dots & \frac{\partial x_n(t; x_0(c))}{\partial c_{n-m}} \end{pmatrix}}_{\frac{\partial x(t, x_0(c))}{\partial c}} \end{aligned}$$

The initial conditions for this differential system are

$$\frac{\partial x(0; x_0(c))}{\partial c_i} = e_{m+i} \quad i \in \{1, 2, \dots, n - m\}, \quad (7)$$

where  $e_{m+i}$  is the notation of the vector of the canonical base from  $\mathbb{R}^n$ .

The two initial value problems are integrated simultaneously

$$\begin{bmatrix} \dot{x}(t) \\ \frac{d}{dt} \frac{\partial x(t; x_0(c))}{\partial c_i} \end{bmatrix} = \begin{bmatrix} f(t, x(t)) \\ f'(t, x(t; x_0(c))) \frac{\partial x(t; x_0(c))}{\partial c_i} \end{bmatrix}, \quad (8)$$

with the initial conditions

$$\begin{bmatrix} x(0, x_0(c)) \\ \frac{\partial x(0; x_0(c))}{\partial c_i} \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} y_0 \\ c \end{bmatrix} \\ e_{m+i} \end{bmatrix}, \quad i \in \{1, 2, \dots, n-m\}.$$

The last  $n$  rows of a column of the solution in  $T$  is a column of  $\frac{\partial x(t, x_0(c))}{\partial c_i}$ . In total  $n-m$  initial value problems must be solved, for each  $c_i$ .

From the equality

$$\frac{\partial x(t; x_0(c))}{\partial c} = \frac{\partial x(t; x_0(c))}{\partial x_0} (P_0^c)^T$$

it results

$$F'(c) = P_T \frac{\partial x(t; x_0(c))}{\partial x_0} (P_0^c)^T. \quad (9)$$

## 4 The connection with adjoint system

Let the ordinary differential system (1) be given. The following system

$$\dot{p}(t) = -f'_x{}^T(t, x(t))p(t) \quad (10)$$

is called the adjoint differential system to (1) [3]. Here we have used the notation  $f'_x(t, x) = \frac{\partial f(t, x)}{\partial x}$ . A solution of this system is an adjoint function.

We denote by  $p^j(t) = (p_1^j, \dots, p_n^j)^T$  the adjoint function satisfying the initial condition  $p^j(T) = e_j$  and

$$P(t) = [p^1(t) \ p^2(t) \ \dots \ p^n(t)].$$

There is a connection between  $P(0)$  and  $\frac{\partial x(T; x_0)}{\partial x_0}$  :

**Theorem 1.** *The following equality holds*

$$\frac{\partial x(T; x_0)}{\partial x_0} = P(0)^T.$$

*Proof.* We have the equalities

$$\begin{aligned} & \langle p^j(T), \frac{\partial x(T; x_0)}{\partial x_{0,k}} \rangle - \langle p^j(0), \frac{\partial x(0; x_0)}{\partial x_{0,k}} \rangle = \\ & = \int_0^T \frac{d}{dt} \langle p^j(t), \frac{\partial x(t; x_0)}{\partial x_{0,k}} \rangle dt = \\ & = \int_0^T \left( \langle \dot{p}^j(t), \frac{\partial x(t; x_0)}{\partial x_{0,k}} \rangle + \langle p^j(t), \frac{d}{dt} \frac{\partial x(t; x_0)}{\partial x_{0,k}} \rangle \right) dt = \\ & = \int_0^T \left( \langle -f'_x{}^T(t, x(t; x_0))p^j(t), \frac{\partial x(t; x_0)}{\partial x_{0,k}} \rangle + \right. \end{aligned}$$

$$+ \left\langle p^j(t), f'_x(t, x(t; x_0)) \frac{\partial x(t; x_0)}{\partial x_{0,k}} \right\rangle dt = 0.$$

Taking into account the initial conditions,  $p^j(T) = e_j$ ,  $\frac{\partial x(0; x_0)}{\partial x_{0,k}} = e_k$ , it results

$$\frac{\partial x_j(T; x_0)}{\partial x_{0,k}} = p_k^j(0). \quad (11)$$

Then it follows that

$$\frac{\partial x(T; x_0)}{\partial x_0} = \begin{pmatrix} \frac{\partial x_1(t; x_0)}{\partial x_{0,1}} & \cdots & \frac{\partial x_1(t; x_0)}{\partial x_{0,n}} \\ \vdots & & \vdots \\ \frac{\partial x_n(t; x_0)}{\partial x_{0,1}} & \cdots & \frac{\partial x_n(t; x_0)}{\partial x_{0,n}} \end{pmatrix} = \begin{pmatrix} p_1^1(0) & \cdots & p_n^1(0) \\ \vdots & & \vdots \\ p_1^n(0) & \cdots & p_n^n(0) \end{pmatrix} = P(0)^T.$$

□

Using adjoint functions we compute the unknown initial values of the BVP (1)-(2). Let be  $x^*(t), x(t)$  two functions verifying (1) and  $\Delta_x = x^* - x$ . Then

$$\dot{\Delta}_x(t) = \dot{x}^*(t) - \dot{x}(t) = f(t, x^*(t)) - f(t, x(t)) = f'_x(t, x(t))\Delta_x(t) + O(\|\Delta_x(t)\|^2).$$

Neglecting the last term, let  $\delta_x(t)$  be such that

$$\dot{\delta}_x(t) = f'_x(t, x(t))\delta_x(t). \quad (12)$$

If  $p(t)$  is an adjoint function, with similar computations as in the proof of the above theorem we obtain

$$\langle p(T), \delta_x(T) \rangle - \langle p(0), \delta_x(0) \rangle = 0. \quad (13)$$

If  $x^*$  is the solution of the BVP (1)-(2) and  $x$  is an approximation of  $x^*$  then we may suppose that  $x_i^*(0) = x_i(0) = y_{0,i}$  and thus  $\delta_{x,i}(0) = \Delta_{x,i}(0) = 0$ , for any  $i \in \mathcal{J}_0 = \{1, 2, \dots, m\}$ . The components of  $\delta_x$  are denoted by  $\delta_{x,i}, i \in \{1, 2, \dots, n\}$ .

For any  $i \in \mathcal{J}_T$  we set the adjoint function  $p := p^i$  and from (13) we deduce

$$\delta_{x,i}(T) - \sum_{j=1}^{n-m} p_{m+j}^i(0)\delta_{x,m+j}(0) = 0, \quad \forall i \in \mathcal{J}_T,$$

or

$$\sum_{j=1}^{n-m} p_{m+j}^i(0)\delta_{x,m+j}(0) = y_{T,i} - x_i(T), \quad \forall i \in \mathcal{J}_T, \quad (14)$$

and in matrix form

$$\begin{pmatrix} p_{m+1}^{j_1} & \cdots & p_n^{j_1} \\ \vdots & & \vdots \\ p_{m+1}^{j_{n-m}} & \cdots & p_n^{j_{n-m}} \end{pmatrix} \begin{pmatrix} \delta_{x,m+1}(0) \\ \vdots \\ \delta_{x,n}(0) \end{pmatrix} = \begin{pmatrix} y_{T,j_1} - x_{j_1}(T) \\ \vdots \\ y_{T,j_{n-m}} - x_{j_{n-m}}(T) \end{pmatrix}.$$

We have obtained an algebraic linear system with the unknowns  $\delta_{x,m+j}(0)$ ,  $j \in \{1, \dots, n-m\}$ .

We interpret (14) as the needed correction of the initial conditions of  $x$  in order to satisfy the boundary conditions in  $T$ .

Due to the neglecting made to obtain (13) we suppose that  $x_{m+j}(0) + \delta_{x,m+j}(0)$ ,  $j \in \{1, \dots, n-m\}$ , are better approximations for the unknown initial conditions and an iterative scheme must be taken into account. If  $x(t) = x(t; x_0(c^k))$  and  $\delta_{x,m+j}(0) = c_j^{k+1} - c_j^k$ ,  $j \in \{1, 2, \dots, n-m\}$  then (14) is rewritten as

$$P_T P(T)^T (P_0^c)^T (c^{k+1} - c^k) = -F(c^k).$$

Taking into account the Theorem 1 and the equality (9) we regain the Newton-Kantorovich iterations.

## 5 Examples

The choice of the unknown initial values is very important mainly for the success of the numerical integration.

**Example 5.1.** [7]

$$\begin{aligned} y''(t) &= 2y(t)y'(t), & t \in [0, 1] \\ y(0) &= 0 \\ y(1) &= 2 \end{aligned}$$

The solution of this BVP is  $y(t) = a \cdot \tan(at)$ , where  $a \approx 1.0768740$ .

Initial values	Final values
$y(0) = 0$	$y(1) = 2.0000000$
$\frac{dy}{dt}(0) = 1.1596576$	$\frac{dy}{dt}(1) = 5.1596576$

The plot of  $y(t)$  and  $\frac{dy(t)}{dt}$  are given in Fig 1a.

**Example 5.2.** [7]

$$\begin{aligned} f^{(3)} + f f'' - (f')^2 &= 0, & t \in [0, 5] \\ \theta'' + k \theta' f &= 0 \\ f(0) &= 0 \\ f'(0) &= 1 \\ f'(5) &= 0 \\ \theta(0) &= 1 \\ \theta(5) &= 0 \end{aligned}$$

where  $k$  is the Prandtl number. We used  $k = 0.71$ .

For different values of the starting initial values it may find different results:

Case	$c^0$
1	$c = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ -1 \end{pmatrix}$

Initial values	Final values
$f(0) = 0$	$f(1) = 0.9740442$
$f'(0) = 1$	$f'(1) = -1.044D - 15$
$f''(0) = -1.0013962$	$f''(1) = -0.0072487$
$\theta(0) = 1$	$\theta(1) = -7.672D - 16$
$\theta'(0) = -0.4755621$	$\theta'(1) = -0.0283081$

Case	$c^0$
2	$c = \begin{pmatrix} -2 \\ 0 \end{pmatrix}$

Initial values	Final values
$f(0) = 0$	$f(1) = -0.8678587$
$f'(0) = 1$	$f'(1) = 4.820D - 16$
$f''(0) = -1.2108404$	$f''(1) = 0.7142624$
$\theta(0) = 1$	$\theta(1) = -1.419D - 15$
$\theta'(0) = -0.2921733$	$\theta'(1) = -0.3115125$

The plot of the trajectories in the two cases are given in Fig. 1b and Fig. 1c.

**Example 5.3.** [1]

$$u''(t) + e^{u(t)+1} = 0 \quad t \in [0, 1];$$

$$u(0) = u(1) = 0$$

This problem with the Bratu type equation [8] has two solutions

$$u(t) = -2 \ln \frac{\cosh((t - \frac{1}{2})\frac{\theta}{2})}{\cosh \frac{\theta}{4}}$$

where  $\theta$  is a solution of the equation  $\theta = \sqrt{2e} \cosh \frac{\theta}{4}$ . This equation has two solutions  $\theta_1 \approx 3.0362318$  and  $\theta_2 \approx 7.1350055$ .

Case	$c^0$
1	$c = 0$

Initial values	Final values
$u(0) = 0$	$u(1) = 2.072D - 10$
$u'(0) = 1.9447725$	$u'(1) = -1.9447725$

Case	$c^0$
2	$c = 5$

Initial values	Final values
$u(0) = 0$	$u(1) = -2.196D - 08$
$u'(0) = 6.7432737$	$u'(1) = -6.7432738$

The plot of the trajectories in the two cases are given in Fig. 1d and Fig. 1e.

**Example 5.4.** [7]

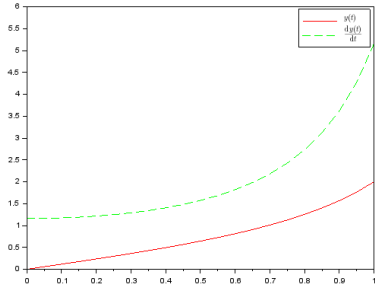
$$\begin{aligned}
 \dot{x}_1(t) &= x_2(t) & t \in [1, 2], \\
 \dot{x}_2(t) &= 2x_1^3(t) - 6x_1(t) - 2t^3 \\
 x_1(1) &= 2 \\
 x_1(2) &= 2.5
 \end{aligned}$$

Initial values	Final values
$x_1(1) = 2$	$x_1(2) = 2.5000000$
$x_2(1) = 6.363D - 10$	$x_2(2) = 0.7500000$

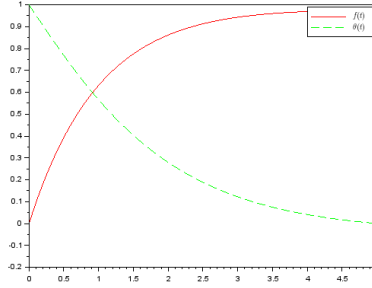
The plot of  $x_1(t)$  and  $x_2(t)$  are given in Fig 1f.

To make the results reproducible we provide some code at <https://github.com/e-scheiber/bvp.git>.

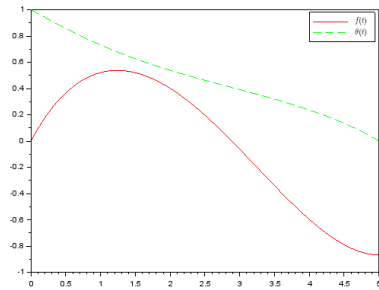




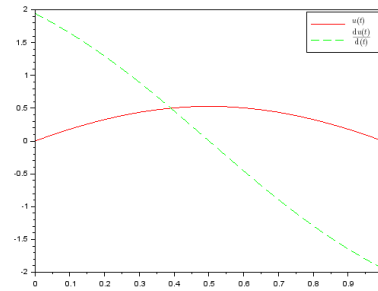
(a) Example 1: Plots of  $y(t)$  and  $\frac{dy(t)}{dt}$ .



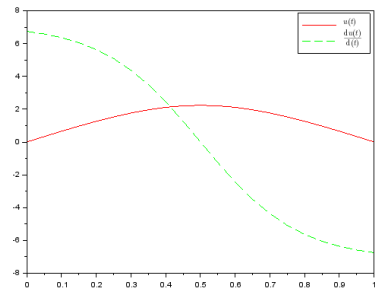
(b) Example 2: Plots of  $f$  and  $\theta$  - case 1.



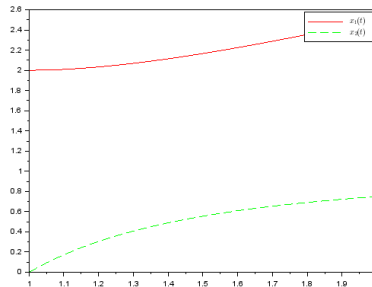
(c) Example 2: Plots of  $f$  and  $\theta$  - case 2.



(d) Example 3: Plots of  $u$  and  $\frac{du(t)}{dt}$  - case 1.



(e) Example 3: Plots of  $u$  and  $\frac{du(t)}{dt}$  - case 2.



(f) Example 4: Plots of  $x_1(t)$  and  $x_2(t)$ .

Figure 1: Graphic representations

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