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ABSTRACT

When solving a boundary value problem for an ordinary differential equation with additional parameters, the usual stability and conditioning concepts induce a more complicated structure; in particular dichotomy of the (linearized) ODE is not necessarily implied. By using the adjoint problem and viewing this as an integral BVP it is shown that the so-called polychotomy of the latter induces a structure for the solution space of the original problem.

1. Introduction

In some applications problems of the following from are met: Let

$$\frac{dx}{dt} = f(x,t,\lambda) , \tag{1.1}$$

with $x : (0,1) \to \mathbb{R}^n$,

be an ODE depending on a vector of parameters $\lambda := (\lambda_1, \cdots, \lambda_m)^T$. For the $m + n$ unknowns there are $m + n$ boundary conditions (BC) specified:

$$g(x(0), x(1), \lambda) = 0 , \tag{1.2}$$

with $g : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^{n \times m}$.

Such problems may e.g. arise in chemistry where the unknown parameters are e.g. reaction rates or in geophysics, where they are wave speeds in different media. Often the BC are even overdetermined, calling for a least squares solution, cf. [1]. Here we shall confine ourselves to the regular case, i.e. we assume that (1.1), (1.2) has an isolated solution. It is natural to think of the solution as the vector y, defined by

$$y(t) := \begin{bmatrix} x(t) \\ \lambda \end{bmatrix} . \tag{1.3}$$

Hence we may augment the ODE (1.1) by

$$\dot{\lambda} = 0 . \tag{1.4}$$

In numerical computations one has to linearize the system (1.1) + (1.4), (1.2) at some stage of a practical algorithm (i.e. before or after discretization); hence one has to solve a sequence of linear BVP for which it makes sense to have knowledge about its conditioning and further structure. As has been shown in [2], linear two point BVP involve ODE having a dichotomic fundamental solution; for multipoint BVP a more complicated structure is present, cf. [4]. This has consequences for a numerical algorithm, in particular for the decoupling of the modes according to their growth behaviour in order to control the stability of the algorithm, cf. [3, 5]. In the sequel we shall show that parameter problems allow for yet another structure. As a consequence numerical methods for such problems should be based on a proper (different) decoupling technique.

2. Structure of the augmented system

When we linearize the ODE (1.1), (1.4) we obtain the following system

$$\frac{dx}{dt} = Lx + C\lambda + r(t) \tag{2.1a}$$

$$\frac{d\lambda}{dt} = 0 , \tag{2.1b}$$

or equivalently using (1.3)

$$\frac{dy}{dt} = \hat{L}y + \hat{r} , \tag{2.1c}$$

Here $L(t) \in \mathbb{R}^{n \times n}$, $C(t) \in \mathbb{R}^{n \times m}$, $\hat{L}(t) \in \mathbb{R}^{(m+n) \times (m+n)}$, $r(t) \in \mathbb{R}^n$, $\hat{r}(t) \in \mathbb{R}^{n+m}$, are all assumed to be continuous at least.

The linearized BC can be written as

$$B_0 x(0) + B_1 x(1) + \tilde{B}_1 \lambda = b \tag{2.2a}$$

$$K_0 x(0) + K_1 x(1) + \tilde{K}_1 \lambda = c , \tag{2.2b}$$

or equivalently

$$\hat{B}_0 y(0) + \hat{B}_1 y(1) = \hat{b} \ . \tag{2.2c}$$

Here $B_0, B_1 \in \mathbb{R}^{n\times n}$, $K_i \in \mathbb{R}^{m\times n}$, $\tilde{B}_1 \in \mathbb{R}^{n\times m}$, $\tilde{K}_1 \in \mathbb{R}^{m\times m}$, $\hat{B}_0, \hat{B}_1 \in \mathbb{R}^{(n+m)\times(n+m)}$. Note that it is not restrictive to assume the last m columns of $\hat{B}_0$ to be zero. Finally, $b \in \mathbb{R}^n$, $c \in \mathbb{R}^m$, $\hat{b} \in \mathbb{R}^{n+m}$.
As is well known, for a well-posed problem, there exist constants κ_1, κ_2, such that

$$\| y \| \le \kappa_1 \| \hat{b} \| + \kappa_2 \| \hat{r} \| \ , \tag{2.3}$$

for appropriate norms (both vector- and function-). For *numerical relevance* these numbers κ_1, κ_2 should actually be *fairly moderate*. We can give an explicit expression for κ_2 based on the Green's function $\hat{G}(t,s)$.
Let $\hat{\Phi}$ be a fundamental solution of (2.1c), and define

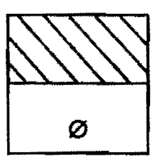
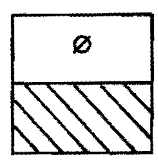
$$\hat{Q} := \hat{B}_0 \hat{\Phi}(0) + \hat{B}_1 \hat{\Phi}(1) \ , \tag{2.4}$$

then

$$\hat{G}(t,s) = \hat{\Phi}(t) \hat{Q}^{-1} \hat{B}_0 \hat{\Phi}(0) \hat{\Phi}^{-1}(s) \ , \qquad t > s \ ; \tag{2.5a}$$

$$\hat{G}(t,s) = -\hat{\Phi}(t) \hat{Q}\, \hat{B}_1 \hat{\Phi}(1) \hat{\Phi}^{-1}(s) \ , \qquad t < s \ . \tag{2.5b}$$

If e.g. the BC are separated, i.e.

(2.6) $\quad \hat{B}_0 \ =$  $\updownarrow l \qquad \hat{B}_1 \ =$  $\updownarrow l$

then the normalisation $\hat{Q} = I$ induces a projection P

$$P = \hat{B}\, \hat{\Phi}(0) = \begin{bmatrix} I_l & \emptyset \\ \emptyset & \emptyset \end{bmatrix} . \tag{2.7}$$

Hence well-conditioning implies

$$\| \hat{\Phi}(t) P\, \hat{\Phi}^{-1}(s) \| \le \kappa_2 \qquad , \qquad t > s \tag{2.8a}$$

$$\| \hat{\Phi}(t) (I - P) \Phi^{-1}(s) \| \le \kappa_2 2, \qquad t > s \ , \tag{2.8b}$$

i.e. the fundamental solution is dichotomic.

Remark 2.9.
In order to appreciate this result one has to realize that κ_2 is moderate indeed. On the other hand, by requiring such a constant κ_2 to be valid uniformly for an entire family of BVP (as in a singular perturbation context), it is clear that such statements can be put in a more mathematically precise framework, like by using asymptotics.

More generally we have

Theorem 2.10.
If the BVP (2.1c), (2.2c) is well-conditioned then there exists a dichotomic fundamental solution, i.e. satisfying (2.8) for some suitable projection P and moderate constant κ_2.

Realizing that $\hat{\Phi}$ can be written as

$$\hat{\Phi}(t) = \begin{bmatrix} \Phi(t) & \varnothing \\ \int_0^t \Phi(s)ds & I \end{bmatrix} * E \ , \tag{2.11}$$

where Φ is a fundamental solution of E and E some nonsingular matrix, we see that dichotomy of $\hat{\Phi}$ does not imply dichotomy as such for Φ. We shall show that this is not true in general either.

3. Integral boundary conditions

In the next section we shall employ results that are known for general BC, including integral BC. As an upshot consider the multipoint BC

$$B_0 x(t_0) + B_1 x(t_1) + \cdots + B_p x(t_p) = b \ , \qquad t_0 = 0 \, , \ t_p = 1 \ . \tag{3.1}$$

By similar arguments as used in the two point case it is straightforward to see that separated BC induce projections and have a structure in the fundamental solution.
In particular we have in a well-conditioned situation that for some fundamental solution Φ and projections $P_0, \cdots, P_p$, with $\sum_{j=0}^{p} P_j = I$, there exists a moderate constant κ such that

$$\| \Phi(t) \left[\sum_{j=0}^{l} P_j \right] \Phi^{-1}(s) \| \le \kappa \quad , \qquad t_l < s < t_{l+1} \, , \ t > s \ , \tag{3.2a}$$

$$\| \Phi(t) \left[\sum_{j=l+1}^{p} P_j \right] \Phi^{-1}(s) \| \le \kappa \ , \qquad t_l < s < t_{l+1} \, , \ t < s \ . \tag{3.2b}$$

In [4] such a fundamental solution was called *polychotomic*.
Note that Φ is dichotomic intervalwise, but that this dichotomy may differ per interval.
Such a polychotomy holds for fairly general BC, cf. [4], such as integral BC

$$\int_0^1 B(t) x(t) dt = b \ , \tag{3.3a}$$

or a combination

$$\int_0^1 B(t)x(t)\,dt + B_0 x(0) + B_1 x(1) = b \ . \tag{3.3b}$$

For interest of us is the form of the Green's function for (3.3b). Given the ODE

$$\frac{dx}{dt} = Lx \ , \tag{3.4}$$

we have

$$G(t,s) = \Phi(t)Q^{-1}\left\{B_0\Phi(0) + \int_0^s B(\tau)\Phi(\tau)\,d\tau\right\}\Phi^{-1}(s) \ , \qquad t > s \tag{3.5a}$$

$$G(t,s) = -\Phi(t)Q^{-1}\left\{B_1\Phi(1) + \int_s^1 B(\tau)\Phi(\tau)\,d\tau\right\}\Phi^{-1}(s) \ , \qquad t < s \ , \tag{3.5b}$$

where

$$Q := B_0\Phi(0) + B_1\Phi(1) + \int_0^1 B(\tau)\Phi(\tau)\,d\tau \ . \tag{3.6}$$

4. The adjoint of the parameter problem

As will turn out we can write the adjoint of our problem (2.1), (2.2) as a BVP with integral BC and hence relate its structure to that of our original problem. To see this we first consider the BC matrices $\hat{B}_0$, $\hat{B}_1$ and write them as an $(n+m) \times (2(n+m))$ matrix:

(4.1)

B_0	$\varnothing$	B_1	$\tilde{B}_1$
K_0	$\varnothing$	K_1	$\tilde{K}_1$

It is not restrictive to assume that $[\hat{B}_0 \mid \hat{B}_1]$ has orthonormal rows. Hence we can construct matrices $\hat{M}_0$ and $\hat{M}_1$ such that

$$\begin{bmatrix} \hat{B}_0 & \hat{B}_1 \\ \hat{M}_0 & \hat{M}_1 \end{bmatrix} \tag{4.2a}$$

is orthogonal. It follows that $[\hat{M}_0 \mid \hat{M}_1]$ has the structure (where we have collected systematic zeros in a manner that suits our purposes):

$$[\hat{M}_0 \mid \hat{M}_1] = \left[\begin{array}{cc|cc} M_0 & \varnothing & M_1 & L_1 \\ \hline \varnothing & L_0 & \varnothing & \varnothing \end{array}\right] . \tag{4.2b}$$

The (homogeneous) adjoint problem of (2.1c), (2.2c) then reads

$$\frac{dz}{dt} = -\hat{L}^T z \tag{4.3}$$

$$\hat{M}_0 z(0) - \hat{M}_1 z(1) = \hat{d} \qquad \text{(for some } \hat{d} \in \mathbb{R}^{n+m}\text{)} . \tag{4.4}$$

Partitioning z and $\hat{d}$ as

$$z = \begin{bmatrix} u \\ v \end{bmatrix} \begin{matrix} \updownarrow n \\ \updownarrow m \end{matrix} , \qquad \hat{d} = \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} \begin{matrix} \updownarrow n \\ \updownarrow m \end{matrix} , \tag{4.5}$$

we see that the system (4.3) is equivalent to

$$\frac{du}{dt} = -L^T u \tag{4.6a}$$

$$\frac{dv}{dt} = -C^T u . \tag{4.6b}$$

The latter ODE is in fact an integral BC for u:

$$v(1) = -\int_0^1 C(\tau)^T u(\tau)\, d\tau + v(0) . \tag{4.6c}$$

The BC (4.4) gives

$$L_0 v(0) = d_2 . \tag{4.7a}$$

Since L_0 must be nonsingular, we find via (4.6c) and (4.7a) the following BC for (4.6a):

$$M_0 u(0) - M_1 u(1) + \int_0^1 L_1 C^T(\tau) u(\tau)\, d\tau = d_1 + L_1 L_0^{-1} d_2 , \tag{4.7b}$$

a BC as in (3.3b).

We now first show that (4.6a), (4.7b) is well-conditioned if (4.3), (4.4) is:

Let Ψ be a fundamental solution of (4.6a), and let Ω be such that

$$\frac{d\Omega}{dt} = -C^T \Psi , \qquad \Omega(0) = 0 . \tag{4.8}$$

Then obviously $\hat{\psi}$ defined by

$$\hat{\Psi} = \begin{bmatrix} \Psi & \varnothing \\ \Omega & I \end{bmatrix} \tag{4.9}$$

is a fundamental solution of (4.3). We obtain (cf. (2.4), (4.4))

$$\hat{Q} := \left[\begin{array}{c|c} M_0\Psi(0) - M_1\Psi(1) - L_1\Omega(1) & -L_1 \\ \hline \varnothing & L_0 \end{array}\right] =: \begin{bmatrix} Q & -L_1 \\ \varnothing & L_0 \end{bmatrix} . \tag{4.10}$$

Denote the Green's function of (4.3), (4.4) by $\hat{H}(t,s)$; then it follows that the $n \times n$ left upper block, $H(t,s)$ say, equals

$$H(t,s) = \Psi(t)\,[Q^{-1} \mid Q^{-1}L_1L_0^{-1}] \begin{bmatrix} M_0\Psi(0)\Psi^{-1}(s) \\ L_0\Omega(s)\Psi^{-1}(s) \end{bmatrix}, \tag{4.11a}$$

$$= \Psi(t)Q^{-1}\left\{M_0\Psi(0) + \int_0^s L_1C^T(\tau)\Psi(\tau)\,d\tau\right\}\Psi^{-1}(s) \ , \quad t > s \ ,$$

$$H(t,s) = -\Psi(t)Q^{-1}\left\{M_1\Psi(1) + \int_s^1 L_1C^T(\tau)\Psi(\tau)\,d\tau\right\}\Psi^{-1}(s) \ , \quad t < s \ . \tag{4.11b}$$

Comparing (4.11) to (3.5) learns that $H(t,s)$ is precisely the Green's function of (4.6a), (4.7b). Now we have

$$\| H(t,s) \| \le \| \hat{H}(t,s) \| \le \max_{t,s} \| \hat{H}(t,s) \| \le \max_{t,s} \| \hat{G}(t,s) \| \le \kappa_2 \ . \tag{4.12}$$

We therefore conclude from § 3 that Ψ is polychotomic.
We have

Property 4.13.
Let Φ, Ψ be fundamental solutions of (2.1a) and (4.6a) respectively. Then $\Psi(t)^T\,\Phi(t)$ is constant.

It is not restrictive to choose Φ such that

$$\Phi(t)^T\,\Psi(t) = I \ . \tag{4.14}$$

Property 4.15.
Let $P_0, \cdots, P_p$ be projections induced by the polychotomy of Ψ (cf. (3.2)). Then

$$\| \Phi(t) \left[\sum_{j=0}^{l} P_j \right] \Phi^{-1}(s) \|_2 = \| \Psi(s) \sum_{j=0}^{l} P_j \Psi^{-1}(t) \|_2 \ .$$

Proof.

$$\Phi(t)\left[\sum_{j=0}^{l} P_j\right]\Phi^{-1}(s) = \Psi^{-T}(t)\left[\sum_{j=0}^{l} P_j\right]\Psi^{-T}(s) .$$

Using the property $\| A^T \|_2 = \| A \|_2$, the result follows. □

Theorem 4.16.

If a linear problem with parameters is well-conditioned then there exist projections $P_0, \cdots, P_p$ *and points* $0 = t_0, \cdots, t_p = 1$, *such that for some moderate constant* κ

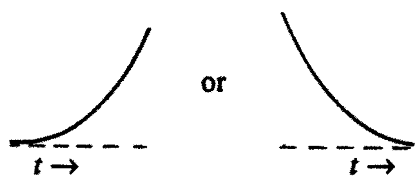
$$\| \Phi(t)\left[\sum_{j=0}^{l} P_j\right]\Phi^{-1}(s) \| \le \kappa \quad , \quad t_l < s < t_{l+1} ,\ t < s , \tag{4.16a}$$

$$\| \Phi(t)\left[\sum_{j=l+1}^{p} P_j\right]\Phi^{-1}(s) \| \le \kappa, \quad t_l < s < t_{l+1} ,\ t > s . \tag{4.16b}$$

We may call the property in (4.16) *skew polychotomy*. Roughly speaking it says that the solution space may be split into subspaces of modes that are nonincreasing till some point t_j after which they become nondecreasing. For clarity one may read for nonincreasing (nondecreasing): decreasing (increasing).

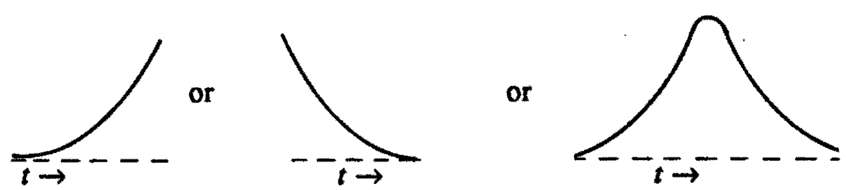
Below we summarize the three types of BVP and the solution types allowed by them:

I **two point:**



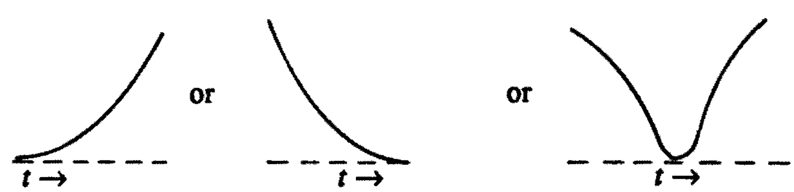
dichotomy

II **integral, multipoint:**



polychotomy

III **parameter:**



skew polychotomy

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