Capstone report 1

Linfan XIAO

Contents

1	Introduction	2
2	Preliminaries[1]	2
	2.1 Green's formula	2
	2.2 Boundary-form formula	7
	2.3 Homogeneous boundary value problem and its adjoint	12
3	Algorithm outline	15
	3.1 Check input	
	3.2 Find U_c	
	3.3 Find U^+	16
	3.4 Check U^+	16
4	Implementation	17
5	Next steps	17

1 Introduction

Solving evolution partial differential equations (PDEs) typically requires ad-hoc methods and special treatments. The recently discovered "Fokas method" [2][3] allows solving many of these equations algorithmically. The first goal of this project concerns implementing the Fokas method in the Julia mathematical programming language. The first steps in the implementation involves constructing a valid adjoint boundary condition from a given homogeneous boundary condition.

Recall from linear algebra that for a linear map T from vector spaces V to W (denoted as $T \in \mathcal{L}(V,W)$), the adjoint of T is the function $T^*:W\to V$ with $\langle Tv,w\rangle=\langle v,T^*w\rangle$ for $v\in V,\,w\in W[4]$. We will see that a similar notion exists for linear differential operators and boundary value problems in general. The "adjoint" problem mirrors certain properties of the original problem. This property is important to the project in that solutions of an adjoint problem are related to those of the original problem in valuable ways.

The algorithm to construct a valid adjoint boundary condition has been completed and will be the main topic of this report. We begin by introducing the preliminary materials on which the construction algorithm depends. In the spirit of making the report self-contained, cited definitions and theorems are included in the report. Most of them are taken from *Theory of Ordinary Differential Equations*[1], with frequent supplies of the student's own notes to build on existing literature so as to make the results relevant to the construction algorithm.

We then present an outline of the construction algorithm, referencing definitions and theorems introduced in the preliminaries section. The outline is in higher-level, abstract form, with occasional pseudo-code illustrations when deemed necessary.

After that, we briefly discuss the implementation of the algorithm in Julia. The discussion will focus on the characterizations of key mathematical objects, notable features, and user experience.

We will conclude the report with a summary of the progress so far with respect to the plan in the project proposal. This will be followed by a brief discussion of plans for the next steps.

2 Preliminaries[1]

The construction algorithm depends on two important results, namely Green's formula and boundary-form formula. Generally speaking, Green's formula provides a characterization, which, when used in the boundary-form formula, gives rise to the desired construction.

We begin with the Green's formula.

2.1 Green's formula

Definition 2.1. A linear differential operator L of order $n \ (n > 1)$ on interval [a, b] is defined by

$$Lx = p_0 x^{(n)} + p_1 x^{(n-1)} + \dots + p_{n-1} x' + p_n x,$$

where the p_k are complex-valued functions of class C^{n-k} on a closed bounded interval [a, b] (i.e., derivatives $p_k, p'_k, \ldots, p_k^{(n-k)}$ exist on [a, b] and are continuous) and $p_0(t) \neq 0$ on [a, b].

Definition 2.2. Homogeneous boundary conditions refer to a set of equations of the type

$$\sum_{k=1}^{n} (M_{jk} x^{(k-1)}(a) + N_{jk} x^{(k-1)}(b)) = 0 \quad (j = 1, \dots, m)$$
(2.1)

where M_{jk}, N_{jk} are complex constants.

Definition 2.3. A homogeneous boundary value problem concerns finding the solutions of

$$Lx = 0$$

on some interval [a, b] which satisfy some homogeneous boundary conditions (Definition 2.2).

For any homogeneous boundary value problem, an **adjoint problem** refers to the problem of finding the solutions of

$$L^+x := (-1)^n (\bar{p}_0 x)^{(n)} + (-1)^{n-1} (\bar{p}_1 x)^{(n-1)} + \dots + \bar{p}_n x = 0$$

on [a, b] which satisfy some homogeneous boundary conditions that correspond to the conditions associated with the solutions of Lx = 0 in interesting ways. We seek to characterize these boundary conditions in the following sections.

With these definitions, we are ready to introduce Green's formula, the first important result the construction depends on.

Theorem 2.4. (Green's formula) For $u, v \in C^n$ on [a, b],

$$\int_{t_1}^{t_2} (Lu)\bar{v} \, dt - \int_{t_1}^{t_2} u(\overline{L^+v}) \, dt = [uv](t_2) - [uv](t_1)$$
(2.2)

where $a \le t_1 < t_2 \le b$ and [uv](t) is the form in $(u, u', \dots, u^{(n-1)})$ and $(v, v', \dots, v^{(n-1)})$ given by

$$[uv](t) = \sum_{m=1}^{n} \sum_{i+k=m-1} (-1)^{j} u^{(k)}(t) (p_{n-m}\bar{v})^{(j)}(t)$$
(2.3)

Using the form [uv](t), we define an important $n \times n$ matrix B whose entries B_{jk} satisfy

$$[uv](t) = \sum_{j,k=1}^{n} B_{jk}(t)u^{(k-1)}(t)\bar{v}^{(j-1)}(t).$$
(2.4)

Note that

$$[uv](t) = \sum_{m=1}^{n} \sum_{j+k=m-1}^{n} (-1)^{j} u^{(k)}(t) (p_{n-m}\bar{v})^{(j)}(t)$$

$$= \sum_{m=1}^{n} \sum_{j+k=m-1}^{n} (-1)^{j} u^{(k)}(t) \left(\sum_{l=0}^{j} {j \choose l} p_{n-m}^{(j-l)}(t) \bar{v}^{(l)}(t)\right)$$

$$= \sum_{m=1}^{n} \sum_{k=0}^{m-1} (-1)^{m-1-k} u^{(k)}(t) \left(\sum_{l=0}^{m-1-k} {m-1-k \choose l} p_{n-m}^{(m-1-k-l)}(t) \bar{v}^{(l)}(t)\right)$$

$$= \sum_{m=1}^{n} \sum_{k=1}^{m} (-1)^{m-k} \left(\sum_{l=0}^{m-k} {m-k \choose l} p_{n-m}^{(m-k-l)}(t) \bar{v}^{(l)}(t)\right) u^{(k-1)}(t) \quad \text{(shifting } k \text{ to } k+1)$$

$$= \sum_{k=1}^{n} \sum_{m=k}^{n} (-1)^{m-k} \left(\sum_{l=0}^{m-k} {m-k \choose l} p_{n-m}^{(m-k-l)}(t) \bar{v}^{(l)}(t)\right) u^{(k-1)}(t).$$

To find B_{jk} , we need to extract the coefficients of $u^{(k-1)}\bar{v}^{(j-1)}$. We first note that, fixing m and k, when l=j-1, the coefficient of $\bar{v}^{(j-1)}$ is

$$\binom{m-k}{j-1}p_{n-m}^{(m-k-j+1)}(t).$$

To find the coefficient of $u^{(k-1)}\bar{v}^{(j-1)}$, we need to fix k and collect the above coefficient across all values of m. Since m goes up to n, m-k goes up to n-k. Since $l \leq m-k, \ l=j-1$ implies $j-1 \leq m-k$. Thus, m-k ranges from j-1 to n-k. Let l':=m-k, then m=k+l', and the above equation becomes

$$[uv](t) = \sum_{k=1}^{n} \sum_{j=1}^{n} (-1)^{l'} \left(\sum_{l'=j-1}^{n-k} {l' \choose j-1} p_{n-(k+l')}^{(l'-(j-1))}(t) \right) \bar{v}^{(j-1)}(t) u^{(k-1)}(t)$$

$$= \sum_{j,k=1}^{n} \left(\sum_{l=j-1}^{n-k} {l \choose j-1} p_{n-k-l}^{(l-j+1)}(t)(-1)^{l} \right) u^{(k-1)}(t) \bar{v}^{(j-1)}(t) \quad \text{(replace } l' \text{ by } l).$$

Thus,

$$B_{jk}(t) = \sum_{l=j-1}^{n-k} {l \choose j-1} p_{n-k-l}^{(l-j+1)}(t)(-1)^{l}.$$

We note that for j+k > n+1, or j-1 > n-k, l is undefined. This means that terms $u^{(k-1)}(t)\bar{v}^{(j-1)}(t)$ with j+k > n+1 does not exist in [uv](t). Thus, $B_{jk}(t) = 0$. Also, for j+k = n+1, or j-1 = n-k,

$$B_{jk}(t) = {j-1 \choose j-1} p_{j-1-(j-1)}^{(j-1-j+1)}(t)(-1)^{j-1} = (-1)^{j-1} p_0(t).$$

Thus, the matrix B has the form

$$B(t) = \begin{bmatrix} B_{11} & B_{12} & \cdots & p_0(t) \\ \vdots & \vdots & \cdots & -p_0(t) & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ (-1)^{n-1}p_0(t) & 0 & \cdots & 0 & 0 \end{bmatrix}.$$
 (2.5)

We note that because $p_0(t) \neq 0$ on [a, b] (as required in Definition 2.1), B(t) is square with det $B(t) = (p_0(t))^n \neq 0$ on [a, b]. Thus, B(t) is nonsingular for $t \in [a, b]$.

Now we seek another matrix B that embodies both the characteristics of B and those of the interval [a,b]. This concerns writing an equation of [uv](t) in matrix form. We begin by introducing the following definitions.

Definition 2.5. For vectors $f = (f_1, \ldots, f_k), g = (g_1, \ldots, g_k),$ define the product

$$f \cdot g := \sum_{i=1}^{k} f_i \bar{g}_i.$$

Note that $f \cdot g = g^* f$.

Definition 2.6. A semibilinear form is a complex-valued function S defined for pairs of vectors $f = (f_1, \ldots, f_k), g = (g_1, \ldots, g_k)$ satisfying

$$S(\alpha f + \beta g, h) = \alpha S(f, h) + \beta S(g, h)$$

$$S(f, \alpha g + \beta h) = \bar{\alpha} S(f, g) + \bar{\beta} S(f, h)$$

for any complex numbers α, β and vectors f, g, h.

We note that if

$$S = \begin{bmatrix} s_{11} & \cdots & s_{1k} \\ \vdots & & \vdots \\ s_{k1} & \cdots & s_{kk} \end{bmatrix},$$

then $Sf \cdot g$ is a semibilinear form given by

$$S(f,g) := Sf \cdot g = \begin{bmatrix} s_{11} & \cdots & s_{1k} \\ \vdots & & \vdots \\ s_{k1} & \cdots & s_{kk} \end{bmatrix} \begin{bmatrix} f_1 \\ \vdots \\ f_k \end{bmatrix} \cdot \begin{bmatrix} g_1 \\ \vdots \\ g_k \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^k s_{1j} f_j \\ \vdots \\ \sum_{j=1}^k s_{kj} f_j \end{bmatrix} \cdot \begin{bmatrix} g_1 \\ \vdots \\ g_k \end{bmatrix}$$

$$= \sum_{i=1}^k \left(\sum_{j=1}^k s_{ij} f_j \right) \bar{g}_i = \sum_{i,j=1}^k s_{ij} f_i \bar{g}_i.$$

$$(2.6)$$

Indeed:

$$S(\alpha f + \beta g, h) = \sum_{i,j=1}^{k} s_{ij} (\alpha f_j + \beta g_j) \bar{h}_i = \alpha \sum_{i,j=1}^{k} s_{ij} f_j \bar{h}_i + \beta \sum_{i,j=1}^{k} g_j \bar{h}_i$$
$$= \alpha S f \cdot h + \beta S g \cdot h = \alpha S(f, h) + \beta S(g, h).$$

Similarly,

$$S(f, \alpha g + \beta h) = \sum_{i,j=1}^{k} s_{ij} f_j (\overline{\alpha g_i + \beta h_i}) = \bar{\alpha} \sum_{i,j=1}^{k} s_{ij} f_j \bar{g}_i + \bar{\beta} \sum_{i,j=1}^{k} f_j \bar{h}_i$$
$$= \bar{\alpha} S f \cdot g + \bar{\beta} S f \cdot h = \bar{\alpha} S(f, g) + \bar{\beta} S(f, h).$$

Under a similar matrix framework, we see that [uv](t) is a semibilinear form with matrix B(t): Let $\vec{u} = (u, u', \dots, u^{(n-1)})$ and $\vec{v} = (v, v', \dots, v^{(n-1)})$. Then we have

$$[uv](t) = \sum_{j,k=1}^{n} B_{jk}(t)u^{(k-1)}(t)\bar{v}^{(j-1)}(t) \quad \text{(by (2.4))}$$

$$= \sum_{i,j=1}^{n} (B_{ij}u^{(j-1)}\bar{v}^{(i-1)})(t)$$

$$= (B\vec{u}\cdot\vec{v})(t) \quad \text{(by (2.6))}$$

$$=: \mathcal{S}(\vec{u},\vec{v})(t).$$

With this notation, we can rewrite the right hand side of Green's formula as a semibilinear form below:

$$[uv](t_2) - [uv](t_1) = \sum_{j,k=1}^{n} B_{jk}(t_2)u^{(k-1)}(t_2)\bar{v}^{(j-1)}(t_2) - \sum_{j,k=1}^{n} B_{jk}(t_2)u^{(k-1)}(t_1)\bar{v}^{(j-1)}(t_1)$$

$$= B(t_2)\bar{u}(t_2) \cdot \bar{v}(t_2) - B(t_1)\bar{u}(t_1) \cdot \bar{v}(t_1)$$

$$= \begin{bmatrix} B_{11}(t_2) & \cdots & B_{1n}(t_2) \\ \vdots & \vdots & \vdots \\ B_{n1}(t_2) & \cdots & B_{nn}(t_2) \end{bmatrix} \begin{bmatrix} u(t_2) \\ \vdots \\ u^{(n-1)}(t_2) \end{bmatrix} \cdot \begin{bmatrix} \bar{v}(t_2) \\ \vdots \\ \bar{v}^{(n-1)}(t_2) \end{bmatrix} - \begin{bmatrix} B_{11}(t_1) & \cdots & B_{1n}(t_1) \\ \vdots & \vdots & \vdots \\ B_{n1}(t_1) & \cdots & B_{nn}(t_1) \end{bmatrix} \begin{bmatrix} u(t_1) \\ \vdots \\ u^{(n-1)}(t_1) \end{bmatrix} \cdot \begin{bmatrix} \bar{v}(t_1) \\ \vdots \\ \bar{v}^{(n-1)}(t_1) \end{bmatrix}$$

$$= \begin{bmatrix} -B_{11}(t_1) & \cdots & -B_{1n}(t_1) \\ \vdots & \vdots & \vdots \\ -B_{n1}(t_1) & \cdots & -B_{nn}(t_1) \end{bmatrix} \begin{bmatrix} u(t_1) \\ u^{(n-1)}(t_1) \end{bmatrix} \cdot \begin{bmatrix} \bar{v}(t_1) \\ \vdots \\ \bar{v}^{(n-1)}(t_1) \end{bmatrix} + \begin{bmatrix} B_{11}(t_2) & \cdots & B_{1n}(t_2) \\ \vdots & \vdots & \vdots \\ B_{n1}(t_2) & \cdots & B_{nn}(t_2) \end{bmatrix} \begin{bmatrix} u(t_2) \\ \vdots \\ u^{(n-1)}(t_1) \end{bmatrix} \cdot \begin{bmatrix} \bar{v}(t_2) \\ \vdots \\ \bar{v}^{(n-1)}(t_2) \end{bmatrix}$$

$$= \begin{bmatrix} -B_{11}(t_1) & \cdots & -B_{1n}(t_1) & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & B_{11}(t_2) & \cdots & B_{1n}(t_2) \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & B_{nn}(t_2) \end{bmatrix} \cdot \begin{bmatrix} \bar{v}(t_1) \\ \vdots \\ \bar{v}^{(n-1)}(t_1) \end{bmatrix}$$

$$= \begin{bmatrix} -B_{11}(t_1) & 0_n \\ 0 & \cdots & 0 & B_{nn}(t_2) & \cdots & B_{nn}(t_2) \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & B_{nn}(t_2) & \cdots & B_{nn}(t_2) \end{bmatrix} \cdot \begin{bmatrix} \bar{v}(t_1) \\ \vdots \\ \bar{v}^{(n-1)}(t_1) \end{bmatrix}$$

$$= \begin{bmatrix} -B(t_1) & 0_n \\ 0_n & B(t_2) \end{bmatrix} \begin{bmatrix} u(t_1) \\ \vdots \\ u^{(n-1)}(t_1) \\ u(t_2) \\ \vdots \\ u^{(n-1)}(t_2) \end{bmatrix} \cdot \begin{bmatrix} \bar{v}(t_1) \\ \vdots \\ \bar{v}(t_2) \\ \vdots \\ \bar{v}^{(n-1)}(t_1) \end{bmatrix}$$

$$= : \hat{B} \begin{bmatrix} \bar{u}(t_1) \\ \bar{u}(t_2) \end{bmatrix} \cdot \begin{bmatrix} \bar{v}(t_1) \\ \bar{v}(t_2) \\ \vdots \\ \bar{v}(t_{n-1})(t_{2}) \end{bmatrix}$$

Recall that $det(\lambda A) = \lambda^n det(A)$ for $n \times n$ matrix A. Thus,

$$\det \hat{B} = \det(-B(t_1)) \det(B(t_2)) = (-1)^n \det B(t_1) \det B(t_2)$$

since $B(t_1)$ is $n \times n$. Since B(t) is nonsingular for $t \in [a, b]$ (as shown before), \hat{B} is nonsingular for $t_1, t_2 \in [a, b]$.

To recapitulate, given a linear differential operator L which involves functions p_0, \ldots, p_n and an interval [a, b], from the Green's formula, we have defined a matrix B which depends on p_0, \ldots, p_n

and a matrix \hat{B} which depends on B and [a, b]. These objects are important constructing an adjoint boundary condition using the boundary-form formula, which we now turn to.

2.2 Boundary-form formula

Before introducing the boundary-form formula, we need a set of definitions and results concerning boundary conditions.

Definition 2.7. Given any set of 2mn complex constants M_{ij} , N_{ij} (i = 1, ..., m; j = 1, ..., n), define m boundary operators (boundary forms) $U_1, ..., U_m$ for functions x on [a, b], for which $x^{(j)}$ (j = 1, ..., n - 1) exists at a and b, by

$$U_{i}x = \sum_{i=1}^{n} (M_{ij}x^{(j-1)}(a) + N_{ij}x^{(j-1)}(b)) \quad (i = 1, \dots, m)$$
(2.9)

 U_i are linearly independent if the only set of complex constants c_1, \ldots, c_m for which

$$\sum_{i=1}^{m} c_i U_i x = 0$$

for all $x \in C^{n-1}$ on [a, b] is $c_1 = c_2 = \cdots = c_m = 0$.

Definition 2.8. A vectory boundary form $U = (U_1, ..., U_m)$ is a vector whose components are boundary forms (Definition 2.7). When $U_1, ..., U_m$ are linearly independent, we say that U has rank m. We assume U has full rank below.

With the above definitions, we can now write a set of homogeneous boundary conditions (Definition 2.2) in matrix form. Define

$$\xi := \begin{bmatrix} x \\ x' \\ \vdots \\ x^{(n-1)} \end{bmatrix}; \quad U := \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_m \end{bmatrix}; \quad M := \begin{bmatrix} M_{11} & \cdots & M_{1n} \\ \vdots & & \vdots \\ M_{m1} & \cdots & M_{mn} \end{bmatrix}; \quad N := \begin{bmatrix} N_{11} & \cdots & N_{1n} \\ \vdots & & \vdots \\ N_{m1} & \cdots & N_{mn} \end{bmatrix}.$$

Then the set of homogeneous boundary conditions in (2.1) can be written as

$$Ux = M\xi(a) + N\xi(b).$$

Indeed:

$$M\xi(a) + N\xi(b) = \begin{bmatrix} M_{11} & \cdots & M_{1n} \\ \vdots & & \vdots \\ M_{m1} & \cdots & M_{mn} \end{bmatrix} \begin{bmatrix} x(a) \\ x'(a) \\ \vdots \\ x^{(n-1)}(a) \end{bmatrix} + \begin{bmatrix} N_{11} & \cdots & N_{1n} \\ \vdots & & \vdots \\ N_{m1} & \cdots & N_{mn} \end{bmatrix} \begin{bmatrix} x(b) \\ x'(b) \\ \vdots \\ x^{(n-1)}(b) \end{bmatrix}$$
$$= \begin{bmatrix} \sum_{j=1}^{n} M_{1j}x^{(j-1)}(a) \\ \vdots \\ \sum_{j=1}^{n} M_{mj}x^{(j-1)}(a) \end{bmatrix} + \begin{bmatrix} \sum_{j=1}^{n} N_{1j}x^{(j-1)}(b) \\ \vdots \\ \sum_{j=1}^{n} N_{mj}x^{(j-1)}(b) \end{bmatrix}$$

$$= \begin{bmatrix} \sum_{j=1}^{n} (M_{1j}x^{(j-1)}(a) + N_{1j}x^{(j-1)}(b)) \\ \vdots \\ \sum_{j=1}^{n} (M_{mj}x^{(j-1)}(a) + N_{mj}x^{(j-1)}(b)) \end{bmatrix}$$
$$= \begin{bmatrix} U_{1}x \\ \vdots \\ U_{m}x \end{bmatrix} = \begin{bmatrix} U_{1} \\ U_{2} \\ \vdots \\ U_{m} \end{bmatrix} x = Ux.$$

Based on the above, we propose another way to write U_x . Define the $m \times 2n$ matrix

$$(M:N) := \begin{bmatrix} M_{11} & \cdots & M_{1n} & N_{11} & \cdots & N_{1n} \\ \vdots & & \vdots & \vdots & & \vdots \\ M_{m1} & \cdots & M_{mn} & N_{m1} & \cdots & N_{mn} \end{bmatrix}.$$

Then U_1, \ldots, U_m are linearly independent if and only if $\operatorname{rank}(M:N) = m$, or equivalently, $\operatorname{rank}(U) = m$. Moreover, Ux can also be written as

$$Ux = \begin{bmatrix} \sum_{j=1}^{n} (M_{1j}x^{(j-1)}(a) + N_{1j}x^{(j-1)}(b)) \\ \vdots \\ \sum_{j=1}^{n} (M_{mj}x^{(j-1)}(a) + N_{mj}x^{(j-1)}(b)) \end{bmatrix}$$

$$= \begin{bmatrix} M_{11} & \cdots & M_{1n} & N_{11} & \cdots & N_{1n} \\ \vdots & & \vdots & & \vdots \\ M_{m1} & \cdots & M_{mn} & N_{m1} & \cdots & N_{mn} \end{bmatrix} \begin{bmatrix} x(a) \\ \vdots \\ x^{(n-1)}(a) \\ x(b) \\ \vdots \\ x^{(n-1)}(b) \end{bmatrix}$$

$$= (M:N) \begin{bmatrix} \xi(a) \\ \xi(b) \end{bmatrix}.$$

Having proposed a compact way to represent a set of homogeneous boundary conditions, we begin building our way to characterizing the notion of adjoint boundary condition. First, we need the notion of complementary boundary form.

Definition 2.9. If $U = (U_1, \ldots, U_m)$ is any boundary form with rank(U) = m and $U_c = (U_{m+1}, \ldots, U_{2n})$ any form with rank $(U_c) = 2n - m$ such that (U_1, \ldots, U_{2n}) has rank 2n, then U and U_c are **complementary boundary forms**.

Note that extending U_1, \ldots, U_m to U_1, \ldots, U_{2n} is equivalent to imbedding the matrix (M:N) in a $2n \times 2n$ nonsingular matrix (recall that a square matrix is nonsingular if and only if it has full rank).

Characterization of adjoint boundary conditions is given by the boundary-form formula. The boundary-form formula is motivated by writing the right-hand side of Green's formula (2.2) as the linear combination of a boundary form U and a complementary form U_c . Before finally getting to it, we first need the following propositions.

Proposition 2.10. In the context of the semibilinear form (2.6), we have

$$Sf \cdot g = f \cdot S^*g, \tag{2.10}$$

where S^* is the conjugate transpose of S.

Proof.

$$Sf \cdot g = \sum_{i,j=1}^{k} s_{ij} f_{j} \bar{g}_{i} \quad \text{(by (2.6))};$$

$$f \cdot S^{*}g = \begin{bmatrix} f_{1} \\ \vdots \\ f_{k} \end{bmatrix} \cdot \begin{bmatrix} \bar{s}_{11} & \cdots & \bar{s}_{k1} \\ \vdots & & \vdots \\ \bar{s}_{1k} & \cdots & \bar{s}_{kk} \end{bmatrix} \begin{bmatrix} g_{1} \\ \vdots \\ g_{k} \end{bmatrix}$$

$$= \begin{bmatrix} f_{1} \\ \vdots \\ f_{k} \end{bmatrix} \cdot \begin{bmatrix} \sum_{j=1}^{k} \bar{s}_{j1} g_{j} \\ \vdots \\ \sum_{j=1}^{k} \bar{s}_{jk} g_{j} \end{bmatrix}$$

$$= \sum_{i=1}^{k} f_{i} \cdot \left(\sum_{j=1}^{k} \bar{s}_{ji} g_{j} \right)$$

$$= \sum_{i,j=1}^{k} f_{i} \cdot \left(\sum_{j=1}^{k} s_{ji} \bar{g}_{j} \right)$$

$$= \sum_{i,j=1}^{k} s_{ji} f_{i} \bar{g}_{j} = Sf \cdot g.$$

Proposition 2.11. Let S be the semibilinear form associated with a nonsingular matrix S. Suppose $\bar{f} := Ff$ where F is a nonsingular matrix. Then there exists a unique nonsingular matrix G such that if $\bar{g} = Gg$, then $S(f,g) = \bar{f} \cdot \bar{g}$ for all f,g.

Proof. Let $G := (SF^{-1})^*$, then

$$S(f,g) = Sf \cdot g$$

$$= S(F^{-1}F)f \cdot g$$

$$= SF^{-1}(Ff) \cdot g$$

$$= SF^{-1}\bar{f} \cdot g$$

$$= \bar{f} \cdot (SF^{-1})^*g \quad (\text{by } (2.10))$$

$$= \bar{f} \cdot G * g$$

$$= \bar{f} \cdot \bar{g}.$$

To see that G is nonsingular, note that $\det G = \det((\overline{SF^{-1}})^T) = \det(\overline{SF^{-1}}) = \overline{\det(SF^{-1})} = \overline{\det(SF^{$

Proposition 2.12. Suppose S is associated with the unit matrix E, i.e., $S(f,g) = f \cdot g$. Let F be a nonsingular matrix such that the first j $(1 \leq j < k)$ components of $\bar{f} = Ff$ are the same as those of f. Then the unique nonsingular matrix G such that $\bar{g} = Gg$ and $\bar{f} \cdot \bar{g} = f \cdot g$ (as in Proposition 2.11) is such that the last k - j components of \bar{g} are linear combinations of the last k - j components of g with nonsingular coefficient matrix.

Proof. We note that for the condition on F to hold, F must have the form

$$\begin{bmatrix} E_j & 0_+ \\ F_+ & F_{k-j} \end{bmatrix}_{k \times k}$$

where E_j is the $j \times j$ identity matrix, 0_+ is the $j \times (k-j)$ zero matrix, F_+ is a $(k-j) \times j$ matrix, and F_{k-j} a $(k-j) \times (k-j)$ matrix. Let G be the unique nonsingular matrix in Proposition 2.11. Write G as

$$\begin{bmatrix} G_j & G_- \\ G_= & G_{k-j} \end{bmatrix}_{k \times k}$$

where $G_j, G_-, G_=, G_{k-j}$ are $j \times j, j \times (k-j), (k-j) \times j, (k-j) \times (k-j)$ matrices, respectively. By the definition of G,

$$f \cdot q = Ff \cdot Gq = \bar{f} \cdot Gq = G^* \bar{f} \cdot q = G^* Ff \cdot q,$$

(where the third equality follows from a reverse application of (2.10) with \bar{f} as f, G^* as S) which implies

$$G^*F = E_k$$
.

Since

$$G^*F = \begin{bmatrix} G_j^* & G_{=}^* \\ G_{-}^* & G_{k-j}^* \end{bmatrix} \begin{bmatrix} E_j & 0_+ \\ F_+ & F_{k-j} \end{bmatrix}$$

$$= \begin{bmatrix} G_j^* + G_{=}^* F_+ & G_{=}^* F_{k-j} \\ G_{-}^* + G_{k-j}^* F_+ & G_{k-j}^* F_{k-j} \end{bmatrix}$$

$$= \begin{bmatrix} E_j & 0_{j \times (k-j)} \\ 0_{(k-j) \times j} & E_{k-j} \end{bmatrix}.$$

Thus, $G_{=}^*F_{k-j}=0_+$, the $j\times (k-j)$ zero matrix. But $\det F=\det(E_j)\cdot\det(F_{k-j})\neq 0$, so $\det F_{k-j}\neq 0$ and we must have $G_{=}^*=0_+$, i.e., $G_{=}=0_{(k-j)\times j}$. Thus, G is upper-triangular, and so $\det G=\det G_j\cdot\det G_{k-j}\neq 0$, which implies $\det G_{k-j}\neq 0$ and G_{k-j} is nonsingular. Hence,

$$\bar{g} = Gg = \begin{bmatrix} G_j & G_- \\ 0_{(k-j)\times j} & G_{k-j} \end{bmatrix} \begin{bmatrix} g_1 \\ \vdots \\ g_k \end{bmatrix}$$

where G_{k-j} is the nonsingular coefficient matrix such that

$$\begin{bmatrix} \bar{g}_{j-1} \\ \vdots \\ \bar{g}_k \end{bmatrix} = G_{k-j} \begin{bmatrix} g_{j-1} \\ \vdots \\ g_k \end{bmatrix}.$$

We are finally ready to introduce the boundary-form formula, the theorem central to the construction of adjoint boundary condition.

Theorem 2.13. (Boundary-form formula) Given any boundary form U of rank m (Definition 2.7), and any complementary form U_c (Definition 2.9), there exist unique boundary forms U_c^+ , U^+ of rank m and 2n - m, respectively, such that

$$[xy](b) - [xy](a) = Ux \cdot U_c^+ y + U_c x \cdot U^+ y. \tag{2.11}$$

If \tilde{U}_c is any other complementary form to U, and $\tilde{U}_c^+, \tilde{U}^+$ the corresponding forms of rank m and 2n-m, then

$$\tilde{U}^{+}y = C^{*}U^{+}y \tag{2.12}$$

for some nonsingular matrix C.

Remark 2.14. U^+ is the key object which will be defined later as an adjoint boundary condition to U. Note that the existence of [xy](t) implies that a linear differential operator is involved (see (2.3)). The matrices \hat{B} and B in the proof also depend on this linear differential operator.

Proof. Recall from (2.8) that the left hand side of (2.11) can be considered as a semibilinear form $S(f,g) = \hat{B}f \cdot g$ for vectors

$$f = \begin{bmatrix} x(a) \\ \vdots \\ x^{(n-1)}(a) \\ x(b) \\ \vdots \\ x^{(n-1)}(b) \end{bmatrix}, g = \begin{bmatrix} y(a) \\ \vdots \\ y^{(n-1)}(a) \\ y(b) \\ \vdots \\ y^{(n-1)}(b) \end{bmatrix}$$

with the nonsingular matrix

$$\hat{B} = \begin{bmatrix} -B(a) & 0_n \\ 0_n & B(b) \end{bmatrix},$$

where B is as in (2.5). Recall from a previous discussion that

$$Ux = M\xi(a) + N\xi(b) = (M:N) \begin{bmatrix} \xi(a) \\ \xi(b) \end{bmatrix}$$

for M, N, ξ are as defined there. With the definition of f, we have $f = \begin{bmatrix} \xi(a) \\ \xi(b) \end{bmatrix}$ and thus

$$Ux = (M:N)f$$
.

By Definition 2.9, $U_c x = (\tilde{M} : \tilde{N}) f$ for two appropriate matrices \tilde{M}, \tilde{N} for which

$$H = \begin{bmatrix} M & N \\ \tilde{M} & \tilde{N} \end{bmatrix}_{2n \times 2n}$$

has rank 2n. Thus,

$$\begin{bmatrix} Ux \\ U_cx \end{bmatrix} = \begin{bmatrix} (M:N)f \\ (\tilde{M}:\tilde{N})f \end{bmatrix} = \begin{bmatrix} M & N \\ \tilde{M} & \tilde{N} \end{bmatrix} f = Hf.$$

By Proposition 2.11, there exists a unique $2n \times 2n$ nonsingular matrix J (in fact, with $S = \hat{B}$, F = H, J = G, and $G = (SF^{-1})^*$, we have $J = (\hat{B}H^{-1})^*$) such that $S(f,g) = Hf \cdot Jg$. Let U^+, U_c^+ be such that

$$Jg = \begin{bmatrix} U_c^+ y \\ U^+ y \end{bmatrix},$$

then

$$[xy](b) - [xy](a) = \mathcal{S}(f,g) = Hf \cdot Jg = \begin{bmatrix} Ux \\ U_cx \end{bmatrix} \cdot \begin{bmatrix} U_c^+y \\ U^+y \end{bmatrix} = Ux \cdot U_c^+y + U_cx \cdot U^+y.$$

Thus, (2.11) holds.

The second statement in the theorem follows from Proposition 2.12 with Hf and Jg corresponding to f and g.

2.3 Homogeneous boundary value problem and its adjoint

The boundary-form formula allows characterizing the notion of "adjoint" for boundary value problems, whose significance is briefly discussed in the introduction section. In this section, we define the notions of "adjoint" for boundary condition and boundary value problem. We then explore some properties of these adjoints as relevant to the construction algorithm.

Definition 2.15. For any boundary form U of rank m there is associated the homogeneous boundary condition

$$Ux = 0 (2.13)$$

for functions $x \in C^{n-1}$ on [a, b]. If U^+ is any boundary form of rank 2n - m determined as in Theorem 2.13, then the homogeneous boundary condition

$$U^{+}x = 0 (2.14)$$

is an adjoint boundary condition to (2.13).

In connection with the notion of adjoint problem introduced after Definition 2.3, we have the following property of adjoint linear differential operator that mirrors the adjoint of a linear map mentioned in the introduction section.

Proposition 2.16. By Green's formula (2.2) and the boundary-form formula (2.11), for $(u, v) := \int_a^b u\bar{v} dt$,

$$(Lu, v) = (u, L^+v)$$

for all $u \in C^n$ on [a,b] satisfying (2.13) and all $v \in C^n$ on [a,b] satisfying (2.14).

Proof.

$$(Lu, v) - (u, L^+v) = \int_a^b Lu\bar{v} dt - \int_a^b u(\overline{L^+v}) dt$$

$$= [uv](a) - [uv](b) \quad \text{(by Green's formula (2.2))}$$

$$= Uu \cdot U_c^+ v + U_c u \cdot U^+ v \quad \text{(by boundary-form formula (2.11))}$$

$$= 0 \cdot U_c^+ v + U_c u \cdot 0 \quad \text{(by (2.13) and (2.14))}$$

$$= 0.$$

Putting together L, L^+ and U, U^+ , we have the definition of adjoint boundary value problem.

Definition 2.17. If U is a boundary form of rank m, the problem of finding solutions of

$$\pi_m: Lx = 0 \quad Ux = 0$$

on [a,b] is a homogeneous boundary value problem of rank m. The problem

$$\pi_{2n-m}^+: L^+x = 0 \quad U^+x = 0$$

on [a, b] is the adjoint boundary value problem to π_m .

Just like how U is associated with two $m \times n$ matrices M, N, U^+ is associated with two $n \times (2n-m)$ matrices P, Q such that $(P^* : Q^*)$ has rank 2n-m and

$$U^{+}x = P^{*}\xi(a) + Q^{*}\xi(b). \tag{2.15}$$

The following theorem is motivated by characterizing the adjoint condition (2.14) in terms of the matrices M, N, P, Q. For our purpose, it provides a way to check whether a boundary condition is a valid adjoint to a given homogeneous boundary condition using the matrices M, N, P, Q.

Theorem 2.18. The boundary condition $U^+x=0$ is adjoint to Ux=0 if and only if

$$MB^{-1}(a)P = NB^{-1}(b)Q (2.16)$$

where B(t) is the $n \times n$ matrix associated with the form [xy](t) ((??)).

Proof. Let $\eta := (y, y', \dots, y^{(n-1)})$, then $[xy](t) = B(t)\xi(t) \cdot \eta(t)$ by (2.7).

Suppose $U^+x=0$ is adjoint to Ux=0. By definition of adjoint boundary condition (2.14), U^+ is determined as in Theorem 2.13. But by Theorem 2.13, in determining U^+ , there exist boundary forms U_c , U_c^+ of rank 2n-m and m, respectively, such that (2.11) holds.

Put

$$U_c x = M_c \xi(a) + N_c \xi(b)$$
 $\operatorname{rank}(M_c : N_c) = 2n - m$
 $U_c^+ y = P_c^* \eta(a) + Q_c^* \eta(b)$ $\operatorname{rank}(P_c^* : Q_c^*) = m$.

Then by the boundary-form formula (2.11),

$$B(b)\xi(b) \cdot \eta(b) - B(a)\xi(a) \cdot \eta(a) = (M\xi(a) + N\xi(b)) \cdot (P_c^*\eta(a) + Q_c^*\eta(b)) + (M_c\xi(a) + N_c\xi(b)) \cdot (P^*\eta(a) + Q^*\eta(b)).$$

By (2.10),

$$M\xi(a) \cdot P_c^* \eta(a) = P_c M\xi(a) \cdot \eta(a).$$

Thus,

$$B(b)\xi(b) \cdot \eta(b) - B(a)\xi(a) \cdot \eta(a) = (P_cM + PM_c)\xi(a) \cdot \eta(a) + (Q_cM + QM_c)\xi(a) \cdot \eta(b)$$
$$(P_cN + PN_c)\xi(b) \cdot \eta(a) + (Q_cN + QN_c)\xi(b) \cdot \eta(b).$$

Thus, we have

$$P_cM + PM_c = -B(a)$$

$$Q_cM + QM_c = 0_n$$

$$Q_cN + QN_c = B(b).$$

Since det $B(t) \neq 0$ on $t \in [a, b]$, $B^{-1}(a)$, $B^{-1}(b)$ exist, and thus

$$\begin{bmatrix} -B^{-1}(a)P_c & -B^{-1}(a)P \\ B^{-1}(b)Q_c & B^{-1}(b)Q \end{bmatrix} \begin{bmatrix} M & N \\ M_c & N_c \end{bmatrix} = \begin{bmatrix} E_n & 0_n \\ 0_n & E_n \end{bmatrix}.$$

Recall that $\begin{bmatrix} M & N \\ M_c & N_c \end{bmatrix}$ has full rank, which means that it is nonsingular (Definition 2.9). Thus, the two matrices on the left are inverses of each other. So we also have

$$\begin{bmatrix} M & N \\ M_c & N_c \end{bmatrix} \begin{bmatrix} -B^{-1}(a)P_c & -B^{-1}(a)P \\ B^{-1}(b)Q_c & B^{-1}(b)Q \end{bmatrix} = \begin{bmatrix} E_m & 0_+ \\ 0_- & E_{2n-m} \end{bmatrix}.$$

Therefore,

$$-MB^{-1}(a)P + NB^{-1}(b)Q = 0_+,$$

which is (2.16).

Conversely, let U_1^+ be a boundary form of rank 2n-m such that

$$U_1^+ y = P_1^* \eta(a) + Q_1^* \eta(b)$$

for appropriate P_1^* , Q_1^* with rank $(P_1^*:Q_1^*)=2n-m$. Suppose

$$MB^{-1}(a)P_1 = NB^{-1}(b)Q_1 (2.17)$$

holds.

By the fundamental theorem of linear maps[4], if V is finite-dimensional and $T \in \mathcal{L}(V, W)$, then $\dim \ker T = \dim V - \dim \operatorname{range} T$. Suppose A is a $n \times k$ matrix, then $A \in \mathcal{L}(\mathbb{R}^n, \mathbb{R}^k)$. Thus, in a homogeneous system of linear equations Ax = 0, we have $\dim \ker A = \dim A - \dim \operatorname{range} A$. That is, the dimension of solution space $\ker A$ is the difference between the number of unknown variables and the rank of the coefficient matrix, or $\dim \operatorname{range} A$. Therefore, letting u be a $2n \times 1$ vector, there exist exactly 2n - m linearly independent solutions of the homogeneous linear system $(M:N)_{m \times 2n} u = 0$. By (2.17),

$$MB^{-1}(a)P_1 - NB^{-1}(b)Q = 0,$$

and thus

$$(M:N)_{m \times 2n} \begin{bmatrix} B^{-1}(a)P_1 \\ -B^{-1}(b)Q_1 \end{bmatrix}_{2n \times (2n-m)} = 0_{m \times (2n-m)}.$$

So the 2n-m columns of the matrix

$$H_1 := \begin{bmatrix} B^{-1}(a)P_1 \\ -B^{-1}(b)Q_1 \end{bmatrix}$$

are solutions of this system. Since $\operatorname{rank}(P_1^*:Q_1^*)=2n-m$,

$$\operatorname{rank} \begin{bmatrix} P_1 \\ Q_1 \end{bmatrix} = 2n - m.$$

Since B(a), B(b) are nonsingular, rank $(H_1) = 2n - m$.

If $U^+x = P^*\xi(a) + Q^*\xi(b) = 0$ is a boundary condition adjoint to Ux = 0, then the matrix

$$\begin{bmatrix} -B^{-1}(a)P_c & -B^{-1}(a)P \\ B^{-1}(b)Q_c & B^{-1}(b)Q \end{bmatrix}_{2n \times 2n}$$

is nonsingular (because it has inverse $\begin{bmatrix} M & N \\ M_c & N_c \end{bmatrix}$), i.e., it has full rank. Thus, if

$$H = \begin{bmatrix} -B^{-1}(a)P \\ B^{-1}(b)Q \end{bmatrix}_{n \times (2n-m)},$$

then $\operatorname{rank}(H) = 2n - m$. Therefore, by (2.16), the 2n - m columns of H also form 2n = m linearly independent solutions of (M:N)u = 0, as in the case of H_1 . Hence, there exists a nonsingular $(2n - m) \times (2n - m)$ matrix A such that $H_1 = HA$ (change of basis in the solution space). Thus we have

$$\begin{bmatrix} B^{-1}(a)P_1 \\ -B^{-1}(b)Q_1 \end{bmatrix} = H_1 = HA = \begin{bmatrix} B^{-1}(a)PA \\ -B^{-1}(b)QA \end{bmatrix},$$

or $P_1 = PA$, $Q_1 = QA$. Thus,

$$U_1^+ y = P_1^* \eta(a) + Q_1^* \eta(b) = A^* P^* \eta(a) + A^* Q^* \eta(b) = A^* U^+ y.$$

Since A^* is a linear map, $U^+y=0$ implies $A^*U^+y=0$. This implies that $U_1^+y=0$ is an adjoint boundary condition to Ux=0.

To recapitulate, the boundary-form formula (Theorem 2.13) gives us the existence and construction of adjoint boundary condition, and Theorem 2.18 gives us a way to check whether a proposed adjoint boundary condition is valid. Now, we are ready to describe an algorithm to construct a valid adjoint given a homogeneous boundary condition.

3 Algorithm outline

Given a homogeneous boundary value problem on [a, b]

$$Lx = 0$$
 $Ux = 0$

where L is a linear differential operator with order n (Definition 2.1) and U is a vector boundary form $U = (U_1, \ldots, U_n)$ (Definition 2.8). For the purpose of the project, we are only interested in cases where m = n. We seek to construct a valid adjoint boundary condition $U^+x = 0$ (Definition 2.15).

3.1 Check input

We first check that U_1, \ldots, U_n are linearly independent. As noted in a previous discussion, write

$$Ux = M\xi(a) + N\xi(b),$$

then it suffices to check whether $\operatorname{rank}(M:N)=n$. U would be considered an invalid input if $\operatorname{rank}(M:N)\neq n$.

3.2 Find U_c

Recall from Definition 2.9 that extending U_1, \ldots, U_n to U_1, \ldots, U_{2n} (where $(U_{n+1}, \ldots, U_{2n})$ is a complementary boundary form U_c) is equivalent to imbedding (M:N) in a $2n \times 2n$ nonsingular matrix (where the newly added rows constitute (\tilde{M}, \tilde{N}) associated with U_c). We construct this $2n \times 2n$ nonsingular matrix from the identity matrix E_{2n} and (M:N) as follows. We append the rows of E_{2n} one by one to (M:N) and discard any row that does not make the rank of the resulting matrix increase, as shown below.

Algorithm 1: Algorithm to find U_c .

The output from the above algorithm is of the form

$$\begin{bmatrix} M & N \\ E' & E'' \end{bmatrix}_{2n \times 2n}$$

where E', E'' are the first n entries and the last n entries of the retained rows of E_{2n} , respectively. We identify this matrix with the matrix

$$H = \begin{bmatrix} M & N \\ \tilde{M} & \tilde{N} \end{bmatrix}$$

in Theorem 2.13 (where \tilde{M}, \tilde{N} give rise to the complementary boundary form $U_c x = \tilde{M}\xi(a) + \tilde{N}\xi(b)$).

3.3 Find U^+

Recall that the linear differential operator L is characterized by the functions p_0, \ldots, p_n and the interval [a,b]. Let B be as in (2.5) which depends on p_0, \ldots, p_n . Construct \hat{B} from B and [a,b] as in Theorem 2.13. Let $J := (\hat{B}H^{-1})^*$. By Theorem 2.13 and Proposition 2.11, we can identify $(P^* : Q^*)$ with the last n rows of J (that is, identify P^* with the lower-left $n \times n$ submatrix of J and Q^* with the lower-right $n \times n$ submatrix of J) and define U^+ by

$$U^+x = P^*\xi(a) + Q^*\xi(b).$$

Then we have found an adjoint U^+ to U.

3.4 Check U^+

By Theorem 2.18, with

$$Ux = M\xi(a) + N\xi(b), \quad U^{+}x = P^{\star}\xi(a) + Q^{\star}\xi(b),$$

we can check whether the U^+ found above is indeed a valid adjoint to U by checking

$$MB^{-1}(a)P = NB^{-1}(b)Q$$

where B is as in (2.5).

4 Implementation

The above algorithm to find U^+ is currently implemented in Julia 0.6.4, where the main functions and unit tests are each of around 600 lines of code. Key structs (or types, objects as in more traditional object-oriented programming languages) include linear differential operator and vector boundary form. A linear differential operator (Definition 2.1) is characterized by a list of functions p_0, \ldots, p_n satisfying some conditions and a tuple (a, b), where a, b are the endpoints of the interval [a, b]. A vector boundary form (Definition 2.8) is characterized by two $n \times n$ matrices M, N such that $\operatorname{rank}(M : N) = n$. Appropriate tests are implemented to ensure the validity of these objects that would be defined by the user.

In order to enhance workflow transparency and user experience, the implementation also comes with a symbolic math feature, which allows the user to keep track of the various functions in the form of symbolic expression. Without this feature, a function defined as f(x) = x + 1 will be displayed as a general method f in Julia without information for the user as to what it actually is. With symbolic expression, f will be displayed as x + 1. The workflow of symbolic expressions is parallel to that of Julia functions, ensuring that the user is able to view the symbolic expression of any output whenever desired

Finding a valid adjoint boundary condition is as simple as calling one function that takes a linear differential operator, a vector boundary form U corresponding to a homogeneous boundary condition, and a matrix containing derivatives of the functions p_0, \ldots, p_n . Yet in the spirit of maximizing workflow transparency, the implementation also contains a set of smaller functions that cover all outputs of each step in the algorithm.

5 Next steps

With regard to the semester 1 plan in the project proposal, the progress has been on track so far. The only difference being that literature review turns out to be proceeding simultaneously with algorithm implementation, instead of sequentially, as suggested in the plan.

The next steps in the project would be to implement a non-classical transform pair (2.15a to 2.16b in [2]) that can be used to solve (complicated) initial-boundary value problems for which there does not exist a classical transform pair. Looking further ahead, when features associated with calculations are in place, we will begin implementing visualization features informed by what researchers in the field of partial differential equations would be interested in seeing.

References

- [1] Earl A. Coddington and Norman Levinson. Theory of Ordinary Differential Equations. McGraw-Hill Publishing, New York, 1977.
- [2] D. A. Smith and A.S. Fokas. Evolution PDEs and augmented eigenfunctions. Half-line. *Journal of Spectral Theory*, 6(1):185–213, 2016.
- [3] Emine Kesici, Beatrice Pelloni, Tristan Pryer, and David Smith. A numerical implementation of the unified Fokas transform for evolution problems on a finite interval. 2016.
- [4] Sheldon Axler. Linear Algebra Done Right. 1997.