Capstone report 1

Linfan XIAO

1 Introduction

Solving evolution partial differential equations (PDEs) typically requires ad-hoc methods and special treatments. The recently discovered "Fokas method"[1] 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.

In this report, we begin by introducing the preliminary materials used by the construction algorithm. 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*[2], 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 preliminary section. The outline is mostly in higher-level or abstract form, with occasional occurrences of pseudo-code 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[2]

The construction algorithm depends on two important results, namely Green's formula and boundary-form formula. Generally speaking, Green's formula provides a way to characterize a form, 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 ($n > 1$) is defined by

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

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

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

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

$$L^+x := (-1)^n(\bar{p}_0x)^{(n)} + (-1)^{n-1}(\bar{p}_1x)^{(n-1)} + \cdots + \bar{p}_nx = 0$$

on $[a, b]$ which satisfy some homogeneous boundary conditions "complementary" to the conditions associated with the solutions of $Lx = 0$. 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 $[a, b]$,*

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

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

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

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

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

Note that

$$\begin{aligned}
[uv](t) &= \sum_{m=1}^{n} \sum_{j+k=m-1} (-1)^j u^{(k)}(t)(p_{n-m}\bar{v})^{(j)}(t) \\
&= \sum_{m=1}^{n} \sum_{j+k=m-1} (-1)^j u^{(k)}(t) \left(\sum_{l=0}^{j} \binom{j}{l} p_{n-m}^{(j-l)}(t)\bar{v}^{(l)}(t) \right) \\
&= \sum_{m=1}^{n} \sum_{k=0}^{m-1} (-1)^{m-1-k} u^{(k)}(t) \left(\sum_{l=0}^{m-1-k} \binom{m-1-k}{l} p_{n-m}^{(m-1-k-l)}(t)\bar{v}^{(l)}(t) \right) \\
&= \sum_{m=1}^{n} \sum_{k=1}^{m} (-1)^{m-k} \left(\sum_{l=0}^{m-k} \binom{m-k}{l} p_{n-m}^{(m-k-l)}(t)\bar{v}^{(l)}(t) \right) u^{(k-1)}(t) \quad \text{(shifting } k \text{ to } k+1\text{)} \\
&= \sum_{k=1}^{n} \sum_{m=k}^{n} (-1)^{m-k} \left(\sum_{l=0}^{m-k} \binom{m-k}{l} p_{n-m}^{(m-k-l)}(t)\bar{v}^{(l)}(t) \right) u^{(k-1)}(t).
\end{aligned}$$

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

$$\begin{aligned}
[uv](t) &= \sum_{k=1}^{n}\sum_{j=1}^{n}(-1)^{l'}\left(\sum_{l'=j-1}^{n-k}\binom{l'}{j-1}p_{n-(k+l')}^{(l'-(j-1))}(t)\right)\bar{v}^{(j-1)}(t)u^{(k-1)}(t) \\
&= \sum_{j,k=1}^{n}\left(\sum_{l=j-1}^{n-k}\binom{l}{j-1}p_{n-k-l}^{(l-j+1)}(t)(-1)^{l}\right)u^{(k-1)}(t)\bar{v}^{(j-1)}(t) \quad \text{(replace } l' \text{ by } l\text{)}.
\end{aligned}$$

Thus,

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

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 $j-1 = n-k$,

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

Thus, the matrix B has the form

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

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 $\hat{B}$ 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 $\mathcal{S}$ defined for pairs of vectors $f = (f_1, \ldots, f_k)$, $g = (g_1, \ldots, g_k)$ satisfying

$$\begin{aligned}\mathcal{S}(\alpha f + \beta g, h) &= \alpha \mathcal{S}(f, h) + \beta \mathcal{S}(g, h)\\ \mathcal{S}(f, \alpha g + \beta h) &= \bar{\alpha} \mathcal{S}(f, g) + \bar{\beta} \mathcal{S}(f, h)\end{aligned}$$

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

$$\begin{aligned}\mathcal{S}(f, g) := Sf \cdot g = \begin{bmatrix} s_{11} & \cdots & s_{1k} \\ \vdots & & \vdots \\ s_{k1} & \cdots & s_{kk} \end{bmatrix} \begin{bmatrix} f_1 \\ \vdots \\ f_k \end{bmatrix} \cdot \begin{bmatrix} g_1 \\ \vdots \\ g_k \end{bmatrix} &= \begin{bmatrix} \sum_{j=1}^k s_{1j} f_j \\ \vdots \\ \sum_{j=1}^k s_{kj} f_j \end{bmatrix} \cdot \begin{bmatrix} g_1 \\ \vdots \\ g_k \end{bmatrix} \\ = \sum_{i=1}^k \left(\sum_{j=1}^k s_{ij} f_j \right) \bar{g}_i = \sum_{i,j=1}^k s_{ij} f_i \bar{g}_i.\end{aligned} \tag{2.6}$$

Indeed:

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

Similarly,

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

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

$$\begin{aligned}[uv](t) &= \sum_{j,k=1}^n B_{jk}(t) u^{(k-1)}(t) \bar{v}^{(j-1)}(t) \quad \text{(by (2.4))} \\ &= \sum_{i,j=1}^n (B_{ij} u^{(j-1)} \overline{v}^{(i-1)})(t) \\ &= (B\vec{u} \cdot \vec{v})(t) \quad \text{(by (2.6))} \\ &=: \mathcal{S}(\vec{u}, \vec{v})(t).\end{aligned} \tag{2.7}$$

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

$$\begin{aligned}
[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)\vec{u}(t_2) \cdot \vec{v}(t_2) - B(t_1)\vec{u}(t_1) \cdot \vec{v}(t_1) \\
&= \begin{bmatrix} B_{11}(t_2) & \cdots & B_{1n}(t_2) \\ \vdots & & \vdots \\ B_{n1}(t_2) & \dots & 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} - \\
&\quad \begin{bmatrix} B_{11}(t_1) & \cdots & B_{1n}(t_1) \\ \vdots & & \vdots \\ B_{n1}(t_1) & \dots & 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 \\ -B_{n1}(t_1) & \dots & -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} + \\
&\quad \begin{bmatrix} B_{11}(t_2) & \cdots & B_{1n}(t_2) \\ \vdots & & \vdots \\ B_{n1}(t_2) & \dots & 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) & 0 & \cdots & 0 \\ \vdots & & \vdots & \vdots & & \vdots \\ -B_{n1}(t_1) & \cdots & -B_{nn}(t_1) & 0 & \cdots & 0 \\ 0 & \cdots & 0 & B_{11}(t_2) & \cdots & B_{1n}(t_2) \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \cdots & 0 & B_{n1}(t_2) & \cdots & B_{nn}(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}^{(n-1)}(t_1) \\ \bar{v}(t_2) \\ \vdots \\ \bar{v}^{(n-1)}(t_2) \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}^{(n-1)}(t_1) \\ \bar{v}(t_2) \\ \vdots \\ \bar{v}^{(n-1)}(t_2) \end{bmatrix} \\
&=: \hat{B} \begin{bmatrix} \vec{u}(t_1) \\ \vec{u}(t_2) \end{bmatrix} \cdot \begin{bmatrix} \vec{v}(t_1) \\ \vec{v}(t_2) \end{bmatrix}.
\end{aligned} \tag{2.8}$$

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 $t_1, t_2 \in [a, b]$.

2.2 Boundary-form formula

We now introduce the definitions and results involving boundary conditions.

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

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

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** $U = (U_1, \ldots, U_m)$ is a vector whose components are boundary forms (Definition 2.7). When $U_1, \ldots, U_m$ 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:

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

$$= \begin{bmatrix} U_1 x \\ \vdots \\ U_m x \end{bmatrix} = \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_m \end{bmatrix} x = Ux.$$

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 $\text{rank}(M : N) = m$, or equivalently, $\text{rank}(U) = m$. Moreover, Ux can also be written as

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

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

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

Having proposed a compact way to represent a set of homogeneous boundary conditions, we begin building our way to characterize the notion of adjoint boundary condition.

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

Note that "appending" $U_{m+1}, \ldots, U_{2n}$ to $U_1, \ldots, U_m$ 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).

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 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.

$$
\begin{aligned}
Sf \cdot g &= \sum_{i,j=1}^{k} s_{ij} f_j \bar{g}_i \quad \text{(by (2.6))}; \\
f \cdot S^* g &= \begin{bmatrix} f_1 \\ \vdots \\ f_k \end{bmatrix} \cdot \begin{bmatrix} \bar{s}_{11} & \cdots & \bar{s}_{k1} \\ \vdots & & \vdots \\ \bar{s}_{1k} & \cdots & \bar{s}_{kk} \end{bmatrix} \begin{bmatrix} g_1 \\ \vdots \\ g_k \end{bmatrix} \\
&= \begin{bmatrix} f_1 \\ \vdots \\ f_k \end{bmatrix} \cdot \begin{bmatrix} \sum_{j=1}^{k} \bar{s}_{j1} g_j \\ \vdots \\ \sum_{j=1}^{k} \bar{s}_{jk} g_j \end{bmatrix} \\
&= \sum_{i=1}^{k} f_i \cdot \overline{\left(\sum_{j=1}^{k} \bar{s}_{ji} g_j \right)} \\
&= \sum_{i=1}^{k} f_i \cdot \left(\sum_{j=1}^{k} s_{ji} \bar{g}_j \right) \\
&= \sum_{i,j=1}^{k} s_{ji} f_i \bar{g}_j = Sf \cdot g.
\end{aligned}
$$

□

Proposition 2.11. *Let $\mathcal{S}$ 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 $\mathcal{S}(f, g) = \bar{f} \cdot \bar{g}$ for all f, g.*

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

$$
\begin{aligned}
\mathcal{S}(f, g) &= Sf \cdot g \\
&= S(F^{-1}F)f \cdot g \\
&= SF^{-1}(Ff) \cdot g \\
&= SF^{-1}\bar{f} \cdot g \\
&= \bar{f} \cdot (SF^{-1})^* g \quad \text{(by (2.10))} \\
&= \bar{f} \cdot G * g \\
&= \bar{f} \cdot \bar{g}.
\end{aligned}
$$

To see that G is nonsingular, note that $\det G = \det((\overline{SF^{-1}})^T) = \det(\overline{SF^{-1}}) = \overline{\det(SF^{-1})} = \overline{\det(S)\det(F)^{-1}} \neq 0$ since S, F are nonsingular. □

Proposition 2.12. *Suppose $\mathcal{S}$ is associated with the unit matrix E, i.e., $\mathcal{S}(f, g) = f \cdot g$. 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,

$$f\cdot g = Ff\cdot Gg = \bar{f}\cdot Gg = G^*\bar{f}\cdot g = G^*Ff\cdot g,$$

(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

$$\begin{aligned} G^*F &= \begin{bmatrix} G_j^* & G_=^* \\ G_-^* & G_{k-j}^* \end{bmatrix}\begin{bmatrix} E_j & 0_+ \\ F_+ & F_{k-j} \end{bmatrix} \\ &= \begin{bmatrix} G_j^* + G_=^*F_+ & G_=^*F_{k-j} \\ G_-^* + G_{k-j}^*F_+ & G_{k-j}^*F_{k-j} \end{bmatrix} \\ &= \begin{bmatrix} E_j & 0_{j\times(k-j)} \\ 0_{(k-j)\times j} & E_{k-j} \end{bmatrix}. \end{aligned}$$

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.

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

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

with the nonsingular matrix

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

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,

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

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 $G = (SF^{-1})^\star$, we have $J = (\hat{B} H^{-1})^\star$) such that $\mathcal{S}(f,g) = Hf \cdot Jg$. Let U^+, U_c^+ be such that

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

then

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

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 gives the existence and definition of adjoint boundary condition, summarized below.

Definition 2.14. For any boundary form U of rank m there is associated the **homogeneous boundary condition**

$$Ux = 0 \tag{2.13}$$

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

$$U^+ x = 0 \tag{2.14}$$

is an **adjoint boundary condition** to 2.13.

In connection with the notion of adjoint homogeneous boundary value problem (Definition **??**), we have the following property of adjoint boundary condition.

Proposition 2.15. *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.

$$\begin{aligned} (Lu, v) - (u, L^+ v) &= \int_a^b Lu\bar{v}\, dt - \int_a^b u(\overline{L^+ v})\, dt \\ &= [uv](a) - [uv](b) \quad \text{(by Green's formula (2.2))} \\ &= Uu \cdot U_c^+ v + U_c u \cdot U^+ v \quad \text{(by boundary-form formula (2.11))} \\ &= 0 \cdot U_c^+ v + U_c u \cdot 0 \quad \text{(by (2.13) and (2.14))} \\ &= 0. \end{aligned}$$

□

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

Definition 2.16. 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

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

Note that imbedding M, N, P^*, Q^* in the same matrix gives

$$\begin{bmatrix} (M : N)_{m \times 2n} \\ (P^* : Q^*)_{(2n-m) \times 2n} \end{bmatrix}_{2n \times 2n} = \begin{bmatrix} M & N \\ P^* & Q^* \end{bmatrix},$$

which is a $2n \times 2n$ matrix of full rank.

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

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

where $B(t)$ is the $n \times n$ matrix associated with the form $[xy](t)$ ((2.5)).

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

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

Then by the boundary-form formula (2.11),

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

By 2.10,

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

Thus,

$$\begin{aligned} B(b)\xi(b) \cdot \eta(b) - B(a)\xi(a) \cdot \eta(a) = (P_c M + P M_c)\xi(a) \cdot \eta(a) + (Q_c M + Q M_c)\xi(a) \cdot \eta(b) \\ (P_c N + P N_c)\xi(b) \cdot \eta(a) + (Q_c N + Q N_c)\xi(b) \cdot \eta(b). \end{aligned}$$

Thus, we have

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

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 $\operatorname{rank}(P_1^* : Q_1^*) = 2n-m$. Suppose

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

holds.

Recall that dim(solution space) + rank(matrix) = # of unknown variables. Let u be a $2n \times 1$ vector, then there exist exactly $2n-m$ linearly independent $2n \times 1$ vector solutions of the 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, $\operatorname{rank}(H_1) = 2n-m$.

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 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 $A^\star$ 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 2.17 gives us a way to check whether a proposed adjoint boundary condition is valid. Now, we are ready to implement an algorithm to construct a valid adjoint given a homogeneous boundary condition.

3 Algorithm outline

Given a homogeneous boundary value problem

$$Lx = 0 \quad Ux = 0$$

where L has order n and $U = (U_1, \dots, U_n)$ (for the purpose of the project, we are only interested in cases where $m = n$), we seek to construct a valid adjoint boundary condition $U^+ x = 0$.

Write

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

3.1 Checking input

We first check that $U_1, \dots, U_n$ are linearly independent. As noted in a previous discussion, thus, we can do so by checking whether rank$(M : N) = n$. U would be considered an invalid input if rank$(M : N) \neq n$.

3.2 Finding U_c

Recall from Definition 2.9 that extending $U_1, \dots, U_n$ to $U_1, \dots, U_{2n}$ is equivalent to imbedding $(M : N)$ in a $2n \times 2n$ nonsingular matrix. 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: Removing rows from $(M : N) : A$ without changing rank: Append and check rank.

Data: $(M : N)_{n\times 2n}$ with rank n, $A_{2n\times 2n}$ with rank $2n$
Result: A $2n \times 2n$ matrix with rank $2n$ where the first n rows are $(M : N)$

```
begin
    mat ⟵ (M : N);
    for i in range(nrow(A)) do
        mat1 ⟵ vcat(mat, A[i,]) ;          ▷ vcat := vertical concatenation
        if rank(mat1) == rank(mat)+1 then
            mat ⟵ mat1
        else
            A ⟵ A[-i,]
    return vcat(mat, A)
```

The output from the above algorithm is of the form

$$\begin{bmatrix} M & N \\ E' & E'' \end{bmatrix}$$

where E', E'' are the first n entries and the last n entries of certain rows of E_{2n}.

We then identify this matrix with

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

and define

$$U_c x = \tilde{M}\xi(a) + \tilde{N}\xi(b).$$

3.3 Finding U^+

Thus, we have found

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

Let $\hat{B}$ be as in 2.8. By Theorem 2.13 and Proposition 2.11, $J = (\hat{B}H^{-1})^*$ is a nonsingular $2n \times 2n$ matrix such that $\mathcal{S}(f, g) = \hat{B}f \cdot g = Hf \cdot Jg$. Let U^+y be the last n rows of Jg. Then we have found U^+.

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 $p_0, \ldots, p_n$ and a tuple (a, b), where a, b are the endpoints of the interval $[a, b]$. A vector boundary form is characterized by two $n \times n$ matrices M, N such that $\text{rank}(M : N) = n$.

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 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 of derivatives corresponding to the functions $p_0, \ldots, p_n$ as arguments. 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

References

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