Algorithmic Solution of High Order Partial Differential Equations in Julia via the Fokas Transform Method

An Initial Thesis Presented in Partial Fulfillment of the Honours Bachelor's Degree in Science

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1 Introduction

Evolution partial differential equations (PDEs) relate a quantity to its rates of change with respect to both time and position. Evolution PDEs can model a variety of phenomena in physics, such as wave propagation and particle motion. This project concerns implementing an algorithmic procedure to solve a certain class of initial-boundary value problems (IBVP) for evolution PDEs in the finite interval [1] based on the Fokas transform method [2]. The implementation is done in Julia, with a focus on symbolic results among numeric features.

1.1 Motivation

To motivate the project, suppose we want to solve some IBVPs.

Certain IBVPs (henceforth referred to as type I problems) can be solved algorithmically via classical transform pairs such as the Fourier transform (Figure 1).
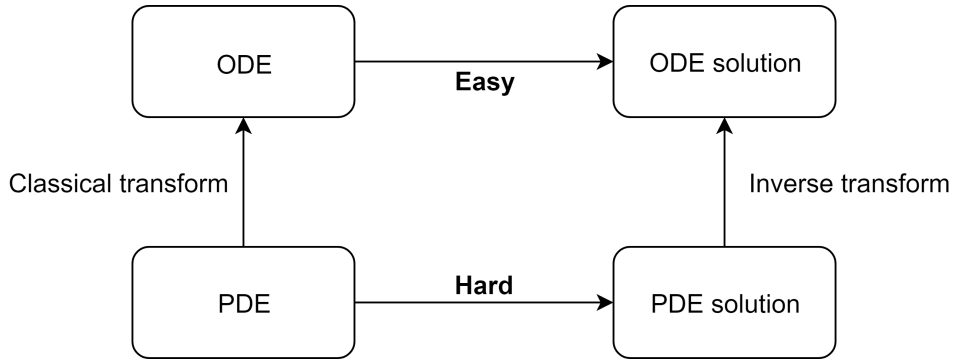
Figure 1: Solving type I IBVPs using classical transform pairs such as the Fourier transform.

For example, the heat equation [3]

$$u_t = au_{xx}, \quad (x,t) \in (0,L) \times (0,\infty)$$

with periodic boundary conditions and initial condition

$$u(0,t) = u(L,t), \quad t \in (0,\infty)$$
$$u_x(0,t) = u_x(L,t), \quad t \in (0,\infty)$$
$$u(x,0) = f(x), \quad x \in (0,L)$$

can be turned into an ordinary differential equation (ODE) in the temporal variable t

$$U_t = -a \cdot s^2 U$$

with initial conditions

$$U(s,0) = F(s), \quad s \in (0,L).$$

where $U(s,t) := \mathcal{F}[u]$ and $F(s) := \mathcal{F}[f]$ are the Fourier transforms of $u(x,t)$ and $f(x)$, respectively, with respect to x. Similarly, the linear Schrödinger equation [4] for a free particle given by

$$ihw_t(x,t) = -\frac{h^2}{2m}w_{xx}(x,t)$$

with periodic boundary conditions can be turned into an ODE

$$W_t(s,t) = \frac{h}{2mi}s^2 W(s,t),$$

where $W(s,t) := \mathcal{F}[w]$ is the Fourier transform of the wave function $w(x,t)$.

For more complicated IBVPs (henceforth referred to as type II problems), however, no such classical transform pairs exist. And solving these IBVPs typically requires a combination of ad-hoc methods. These methods are often specific to the given problem and cannot be generalized to problems with different parameters (e.g., IBVP involving PDE of a different order or different boundary conditions).

The Fokas transform method [2] extends the idea of transform pairs to solving type II problems by constructing non-classical transform pairs based on the problem parameters. Since appropriate transform pairs can now be "customized" for IBVPs with different parameters, this means that the Fokas method allows solving an entire class of IBVPs algorithmically in a manner similar to Figure 1 (Figure 2).
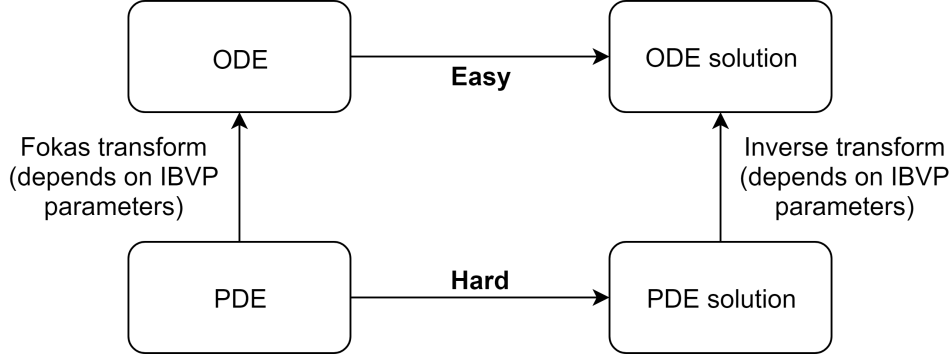

Figure 2: Solving type II IBVPs using the Fokas transform pairs.

Examples of IBVPs that can be solved by the Fokas method include second order PDEs of the form
$$q_t(x,t) + a(-i)^2 q_{xx}(x,t) = 0,$$

with boundary conditions
$$\begin{aligned} q(0,t) + c_0 q(1,t) &= 0 \\ q_x(0,t) + c_1 q_x(1,t) &= 0, \end{aligned} \tag{1.1}$$

or
$$\begin{aligned} q(0,t) + c_0 q_x(0,t) &= 0 \\ q(1) + c_1 q_x(1,t) &= 0, \end{aligned}$$

where $c_0, c_1 \in \hat{\mathbb{C}} := \mathbb{C} \cup \{0, \infty\}$ (in the sense that if $c_0 = \infty$ in 1.1, then dividing by c_0 makes $q(0,t)$ disappear and leaves the first equation as $q(1,t) = 0$), as well as third order PDEs of the form
$$q_t(x,t) \pm i(-i)^2 q_{xxx}(x,t) = 0,$$

with boundary conditions
$$\begin{aligned} q(0,t) + c_0 q(1,t) &= 0 \\ q_x(0,t) + c_1 q_x(1,t) &= 0 \\ q_{xx}(0,t) + c_2 q_{xx}(1,t) &= 0, \end{aligned}$$

where $c_j \in \hat{\mathbb{C}}$ for $j = 0, 1, 2$, or
$$\begin{aligned} q(0,t) &= 0 \\ q(1,t) &= 0 \end{aligned}$$

$$q_x(0, t) + cq_x(1, t) = 0,$$

where $c \in \hat{\mathbb{C}}$.

In fact, as we will see later, the Fokas method is applicable to IBVPs in the above form with PDEs of any general order n. In general, compared to PDEs of higher orders, first and second order PDEs are studied and applied more frequently. The Fokas method advances the understanding of PDEs with higher orders by providing an algorithmic way to solve an entire class of IBVPs of arbitrary order. Using the Fokas method by hand, however, is laborious. It is thus of interest to implement the Fokas method as a software package that aims to supply as much computer aid as possible in the computation process. Examples of such computer aid include visualizations of integration contours, numerical evaluations, and deriving explicit symbolic formulae for important objects which would help proving technical lemmas that arise when applying the Fokas method to different types of problems [5].

This project is developed in Julia, a free open-source, high-performance language for numerical computing [6]. Among tools for numerical computing, commercial softwares may provide functionalities to execute sophisticated computational tasks; yet due to being closed-source, there exists a lack of transparency which limits users' understanding of the nature of the software output. As a result, there has been a trend in the mathematical community that encourages the use of open-source languages like Julia, which allows users to verify the correctness of the output. Therefore, we choose Julia to be the language of implementation. To our knowledge, despite the presence of various differential equation solvers in mathematical softwares such as Mathematica and Matlab, this is the first time that the Fokas method is implemented computationally, which allows solving a particular class of IBVPs for which no other solver algorithm yet exists.

1.2   The Initial-Boundary Value Problem

To formally characterize the class of IBVPs that can be solved by the Fokas method [1, p.9], we first introduce the following definitions.

- Define linearly independent boundary forms $B_j : C^\infty[0, 1] \to \mathbb{C}$ (where $C^\infty[0, 1]$ denotes the class of real-valued functions differentiable for all orders on $[0, 1]$) by

$$B_j\phi := \sum_{k=0}^{n-1} \left(b_{jk}\phi^{(k)}(0) + \beta_{jk}\phi^{(k)}(1) \right), \; j \in \{1, 2, \dots, n\} \tag{1.2}$$

   where the boundary coefficients $b_{jk}, \beta_{jk} \in \mathbb{R}$.

- Define
$$\Phi := \{\phi \in C^\infty[0, 1] : \; B_j\phi = 0 \, \forall j \in \{1, 2, \dots, n\}\} \tag{1.3}$$

   to be the set of smooth functions ϕ satisfying the homogeneous boundary conditions $B_j\phi = 0$ for $j \in \{1, 2, \dots, n\}$.

- Define
$$S = (-i)^n \frac{d^n}{dx^n}$$

   to be a spatial differential operator of order n (i.e., a differential operator in the spatial variable x).

The Fokas method allows solving any well-posed IBVP that can be written in the form

$$(\partial_t + aS)q(x, t) = 0 \qquad \forall (x, t) \in (0, 1) \times (0, T) \tag{1.4}$$

$$q(x, 0) = q_0(x) \in \Phi \qquad \forall x \in [0, 1] \tag{1.5}$$

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$$q(\cdot, t) = f \in \Phi \qquad \forall t \in [0, T], \tag{1.6}$$

where a is a complex constant. For the IBVP to be well-posed, we require that $a = \pm i$ if n is odd and $\text{Re}(a) \geq 0$ if n is even. Equation 1.4 is a PDE relating a quantity q to its temporal and spatial rates of change $\partial_t[q]$ and $aS[q]$. 1.5 is the initial condition where the temporal variable $t = 0$. 1.6 corresponds to the homogeneous spatial boundary conditions. An example of such IBVPs is the linear Schrödinger equation [4], which describes the wave form of a quantum system in free space. The linear Schrödinger equation with zero potential is given by

$$ih\frac{\partial}{\partial t}w + \frac{h^2}{2m}\frac{\partial^2}{\partial x^2}w = 0,$$

where $w(x, t)$ is the wave function, h is the Planck's constant, m is the mass of the particle, and kx describes the potential energy of the particle in the force field. It can be written in the form of 1.4 as

$$(\partial_t + aS)q(x, t) = 0$$

where $q = w$, $S = \frac{\partial^2}{\partial x^2}$, and $a = \frac{h}{2mi}$. The initial condition

$$w(x, 0) = w_0(x)$$

would mean that the system's wave form at initial stage is described by the wave function $w_0(x)$, and the boundary conditions

$$w(\cdot, t) = f$$

would mean that the behaviour of the system at its boundary is described by the function f (e.g., if we are considering particles moving in a box, f would describe how the particles behave at the box's boundaries).

For appropriate transform pair $f(x) = f_x(F)$ and $F(\lambda) = F_\lambda(f)$ found using the Fokas method, the solution to the IBVP characterized above is given by [1, p.15]

$$q(x, t) = f_x(e^{-a\lambda^n t}F_\lambda(f)), \tag{1.7}$$

completing Figure 2.

2 Preliminaries

We now begin to introduce the preliminary definitions and results used in the algorithmic procedure that finds 1.7.

2.1 Homogeneous Boundary Value Problems

Definition 2.1. [7, p.81] A **linear differential operator** L of order n $(n > 1)$ on interval $[a, b]$ is defined by

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

where the p_k are complex-valued functions of class C^{n-k} on $[a, b]$ and $p_0(t) \neq 0$ on $[a, b]$.

Definition 2.2. [7, p.284] **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. [7, p.284] A **homogeneous boundary value problem** concerns finding the solutions of

$$Lx = 0$$

on some interval $[a, b]$ which satisfy some homogeneous boundary conditions.

2.2 Adjoints of Homogeneous Boundary Value Problems

Recall from Linear Algebra that, given a linear map T from inner product spaces V to W (denoted as $T \in \mathcal{L}(V, W)$), the adjoint of T is the function $T^\star : W \to V$ with

$$\langle Tv, w \rangle = \langle v, T^\star w \rangle \tag{2.2}$$

for $v \in V$, $w \in W$, where $\langle \cdot, \cdot \rangle$ denotes inner products defined on V and W [8, p.204]. There exists a similar notion for boundary value problems, which we begin to characterize below.

2.2.1 Adjoint Differential Operator

Definition 2.4. [7, p.84] Given a linear differential operator L of order n as in Definition 2.1, the operator L^+ given by

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

(where $\bar{p}_k$ is the complex conjugate of p_k for $k \in \{0, \ldots, n\}$) is the **adjoint** of L.

2.2.2 Adjoint Boundary Conditions

For a homogeneous boundary value problem π with linear differential operator L and some (homogeneous) boundary conditions, an adjoint problem π^+ involves the adjoint linear differential operator L^+ and some (homogeneous) adjoint boundary conditions. The adjoint boundary conditions are such that an equation similar to (2.2) exists for solutions of π and those of π^+, with the inner product $\langle \cdot, \cdot \rangle$ defined as $\langle u, v \rangle := \int_a^b u \bar{v} \, dt$ for $u, v \in C^n$ on $[a, b]$. In the following sections, we seek to characterize the adjoint boundary conditions.

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

We begin with the Green's formula.

Green's formula

Theorem 2.5. *[7, p.284](Green's formula) For $u, v \in C^n$ on $[a, b]$,*

$$\int_{t_1}^{t_2} (Lu) \bar{v} \, dt - \int_{t_1}^{t_2} u (\overline{L^+ v}) \, dt = [uv](t_2) - [uv](t_1) \tag{2.3}$$

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

$$[uv](t) = \sum_{m=1}^{n} \sum_{j+k=m-1} (-1)^j u^{(k)}(t) (p_{n-m} \bar{v})^{(j)}(t) \tag{2.4}$$

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

$$[uv](t) = \sum_{j,k=1}^{n} B_{jk}(t) u^{(k-1)}(t) \bar{v}^{(j-1)}(t). \tag{2.5}$$

Note that

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

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

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 $\ell = j-1$, 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 $\ell \leq m-k$, $\ell = j-1$ implies $j-1 \leq m-k$. Thus, $m-k$ ranges from $j-1$ to $n-k$. Let $\ell' := m-k$, then $m = k+\ell'$, and the above equation becomes

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

Thus,

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

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

$$
B(t) = \begin{bmatrix}
B_{11} & B_{12} & \cdots & \cdots & B_{1\,n-1} & p_0(t) \\
B_{21} & B_{22} & \cdots & \cdots & -p_0(t) & 0 \\
\vdots & \vdots & \ddots & & \vdots & \vdots \\
\vdots & \vdots & & \ddots & \vdots & \vdots \\
(-1)^{n-1} p_0(t) & 0 & \cdots & \cdots & 0 & 0
\end{bmatrix}. \tag{2.6}
$$

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 the right-hand side of Green's formula in matrix form. We begin by introducing the following definitions.

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Definition 2.6. [7, p.285] 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 $f \cdot g = g^* f$ where $*$ denotes conjugate transpose.

Definition 2.7. [7, p.285] 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

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

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 given by

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

$$= \sum_{i=1}^{k} \left(\sum_{j=1}^{k} s_{ij} f_j \right) \bar{g}_i = \sum_{i,j=1}^{k} s_{ij} f_i \bar{g}_i. \tag{2.7}$$

To see that this is a semibilinear form:

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

$$= \alpha Sf \cdot h + \beta Sg \cdot h = \alpha \mathcal{S}(f, h) + \beta \mathcal{S}(g, h);$$

and similarly,

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

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

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

$$[uv](t) = \sum_{j,k=1}^{n} B_{jk}(t) u^{(k-1)}(t) \bar{v}^{(j-1)}(t) \quad \text{(by (2.5))}$$

$$= \sum_{i,j=1}^{n} (B_{ij} u^{(j-1)} \bar{v}^{(i-1)})(t) \tag{2.8}$$

$$= (B\vec{u} \cdot \vec{v})(t) \quad \text{(by (2.7))}$$

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

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

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

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

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

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

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

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

$$= \begin{bmatrix} -B_{11}(t_1) & \cdots & -B_{1n}(t_1) & 0 & \cdots & 0 \\ \vdots & & \vdots & \vdots & & \vdots \\ -B_{n1}(t_1) & \cdots & -B_{nn}(t_1) & 0 & \cdots & 0 \\ 0 & \cdots & 0 & B_{11}(t_2) & \cdots & B_{1n}(t_2) \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \cdots & 0 & B_{n1}(t_2) & \cdots & B_{nn}(t_2) \end{bmatrix} \begin{bmatrix} u(t_1) \\ \vdots \\ u^{(n-1)}(t_1) \\ u(t_2) \\ \vdots \\ u^{(n-1)}(t_2) \end{bmatrix} \cdot \begin{bmatrix} \bar{v}(t_1) \\ \vdots \\ \bar{v}^{(n-1)}(t_1) \\ \bar{v}(t_2) \\ \vdots \\ \bar{v}^{(n-1)}(t_2) \end{bmatrix}$$

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

$$=: \hat{B} \begin{bmatrix} \vec{u}(t_1) \\ \vec{u}(t_2) \end{bmatrix} \cdot \begin{bmatrix} \vec{v}(t_1) \\ \vec{v}(t_2) \end{bmatrix}.$$

$$(2.9)$$

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 will be important in characterizing an adjoint boundary condition using the boundary-form formula, which we now turn to.

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

Definition 2.8. [7, p.286] 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

$$U_i x = \sum_{j=1}^{n} (M_{ij} x^{(j-1)}(a) + N_{ij} x^{(j-1)}(b)) \quad (i = 1, \ldots, m) \tag{2.10}$$

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 2.9. [7, p.286] A **vectory boundary form** $U = (U_1, \ldots, U_m)$ is a vector whose components are boundary forms (Definition 2.8). 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:

$$
\begin{aligned}
M\xi(a) + N\xi(b) &= \begin{bmatrix} M_{11} & \cdots & M_{1n} \\ \vdots & & \vdots \\ M_{m1} & \cdots & M_{mn} \end{bmatrix} \begin{bmatrix} x(a) \\ x'(a) \\ \vdots \\ x^{(n-1)}(a) \end{bmatrix} + \begin{bmatrix} N_{11} & \cdots & N_{1n} \\ \vdots & & \vdots \\ N_{m1} & \cdots & N_{mn} \end{bmatrix} \begin{bmatrix} x(b) \\ x'(b) \\ \vdots \\ x^{(n-1)}(b) \end{bmatrix} \\
&= \begin{bmatrix} \sum_{j=1}^{n} M_{1j} x^{(j-1)}(a) \\ \vdots \\ \sum_{j=1}^{n} M_{mj} x^{(j-1)}(a) \end{bmatrix} + \begin{bmatrix} \sum_{j=1}^{n} N_{1j} x^{(j-1)}(b) \\ \vdots \\ \sum_{j=1}^{n} N_{mj} x^{(j-1)}(b) \end{bmatrix} \\
&= \begin{bmatrix} \sum_{j=1}^{n} (M_{1j} x^{(j-1)}(a) + N_{1j} x^{(j-1)}(b)) \\ \vdots \\ \sum_{j=1}^{n} (M_{mj} x^{(j-1)}(a) + N_{mj} x^{(j-1)}(b)) \end{bmatrix} \\
&= \begin{bmatrix} U_1 x \\ \vdots \\ U_m x \end{bmatrix} = \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_m \end{bmatrix} x = Ux.
\end{aligned}
$$

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 characterizing the notion of adjoint boundary condition. First, we need the notion of a complementary boundary form.

Definition 2.10. [7, p.287] If $U = (U_1, \ldots, U_m)$ is any boundary form with $\text{rank}(U) = m$ and $U_c = (U_{m+1}, \ldots, U_{2n})$ is 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 extending $U_1, \ldots, U_m$ to $U_1, \ldots, U_{2n}$ is equivalent to embedding 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 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 (2.3) as the linear combination of a boundary form U and a complementary form U_c. Before finally getting to it, we need the following propositions.

Proposition 2.11. *[7, p.287] In the context of the semibilinear form (2.7), we have*

$$Sf \cdot g = f \cdot S^*g, \tag{2.11}$$

where S^* is the conjugate transpose of S.

Proof.

$$Sf \cdot g = \sum_{i,j=1}^{k} s_{ij} f_j \bar{g}_i \quad \text{(by (2.7))};$$

$$f \cdot S^*g = \begin{bmatrix} f_1 \\ \vdots \\ f_k \end{bmatrix} \cdot \begin{bmatrix} \bar{s}_{11} & \cdots & \bar{s}_{k1} \\ \vdots & & \vdots \\ \bar{s}_{1k} & \cdots & \bar{s}_{kk} \end{bmatrix} \begin{bmatrix} g_1 \\ \vdots \\ g_k \end{bmatrix}$$

$$
= \begin{bmatrix} f_1 \\ \vdots \\ f_k \end{bmatrix} \cdot \begin{bmatrix} \sum_{j=1}^{k} \bar{s}_{j1} g_j \\ \vdots \\ \sum_{j=1}^{k} \bar{s}_{jk} g_j \end{bmatrix}
$$

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

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

$$
= \sum_{i,j=1}^{k} s_{ji} f_i \bar{g}_j = Sf \cdot g. \qquad \square
$$

Proposition 2.12. *[7, p.287] 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

$$
\begin{aligned}
\mathcal{S}(f,g) &= Sf \cdot g \\
&= S(F^{-1}F)f \cdot g \\
&= SF^{-1}(Ff) \cdot g \\
&= SF^{-1}\bar{f} \cdot g \\
&= \bar{f} \cdot (SF^{-1})^* g \quad \text{(by (2.11))} \\
&= \bar{f} \cdot G * g \\
&= \bar{f} \cdot \bar{g}.
\end{aligned}
$$

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. $\qquad \square$

Proposition 2.13. *[7, p.287] 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 2.12) 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 2.12. 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,

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

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(where the third equality follows from a reverse application of (2.11) 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

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

$\square$

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

Theorem 2.14. *[7, p.288](Boundary-form formula) Given any boundary form U of rank m (Definition 2.8), and any complementary form U_c (Definition 2.10), there exist unique boundary forms U_c^+, U^+ of rank m and $2n - m$, respectively, such that*

$$[xy](b) - [xy](a) = Ux \cdot U_c^+ y + U_c x \cdot U^+ y. \tag{2.12}$$

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

$$\tilde{U}^+ y = C^* U^+ y \tag{2.13}$$

for some nonsingular matrix C.

Remark 2.15. 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 (2.4)). The matrices $\hat{B}$ and B in the proof also depend on this linear differential operator.

Also note that the second statement in the theorem reflects the fact that adjoint boundary conditions are unique only up to linear transformation. This is why when the need for rigor is greater than that for convenience, we take care to use "an" instead of "the" in referring to adjoint boundary condition.

Proof. Recall from (2.9) that the left-hand side of (2.12) can be considered as a semibilinear form $\mathcal{S}(f,g) = \hat{B}f \cdot g$ for vectors

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

with the nonsingular matrix

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

where B is as in (2.6). 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 2.10, $U_c x = (\tilde{M} : \tilde{N})f$ 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 2.12, there exists a unique $2n \times 2n$ nonsingular matrix J (in fact, with $S = \hat{B}$, $F = H$, $J = G$, and $G = (SF^{-1})^\star$ where * denotes the conjugate transpose, 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, (2.12) holds.

The second statement in the theorem follows from Proposition 2.13 with Hf and Jg corresponding to f and g. $\qquad \square$

Characterization of the Adjoint   With the boundary-form formula, we are now able to fully characterize the notion of "adjoint" for boundary value problems. In this section, we begin by defining adjoint boundary condition and adjoint boundary value problem. We then explore some properties of these adjoints as relevant to the construction algorithm.

Definition 2.16. [7, p.288-89] For any boundary form U of rank m there is associated the homogeneous boundary condition

$$Ux = 0 \qquad (2.14)$$

for functions $x \in C^{n-1}$ on $[a,b]$. If U^+ is any boundary form of rank $2n - m$ determined as in Theorem 2.14, then the homogeneous boundary condition

$$U^+ x = 0 \qquad (2.15)$$

is an **adjoint boundary condition** to (2.14).

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

Definition 2.17. [7, p.291] 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.

In connection with the notion of adjoint problem introduced after Definition 2.3, we now have the following property of the adjoint analogous to (2.2).

Proposition 2.18. *By Green's formula (2.3) and the boundary-form formula (2.12),*

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

for all $u \in C^n$ on $[a,b]$ satisfying (2.14) and all $v \in C^n$ on $[a,b]$ satisfying (2.15).

Proof.

$$
\begin{aligned}
(Lu, v) - (u, L^+ v) &= \int_a^b Lu\bar{v}\, dt - \int_a^b u(\overline{L^+ v})\, dt \\
&= [uv](a) - [uv](b) \quad \text{(by Green's formula (2.3))} \\
&= Uu \cdot U_c^+ v + U_c u \cdot U^+ v \quad \text{(by boundary-form formula (2.12))} \\
&= 0 \cdot U_c^+ v + U_c u \cdot 0 \quad \text{(by (2.14) and (2.15))} \\
&= 0. \qquad\qquad\qquad\qquad\qquad \square
\end{aligned}
$$

Here, we treat the above result as a property of the adjoint after defining L^+ and constructing U^+. In some cases, it is treated as the definition of the adjoint problem, especially if the context wishes to introduce the adjoint problem using linear algebra. Historically, though, it is the adjoint problem that motivated the inner product characterization.

Now, we turn to one last result that would help us in the last step of the construction algorithm, namely checking whether an adjoint boundary condition is valid.

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

$$U^+ x = P^* \xi(a) + Q^* \xi(b). \qquad (2.16)$$

The following theorem is motivated by characterizing the adjoint condition (2.15) in terms of the matrices M, N, P, Q. For our purpose, it provides a way to check whether the adjoint boundary condition found by the algorithm is indeed valid using the matrices M, N, P, Q.

Theorem 2.19. *[7, p.289] The boundary condition $U^+x = 0$ is adjoint to $Ux = 0$ if and only if*

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

where $B(t)$ is the $n \times n$ matrix associated with the form $[xy](t)$ (2.6).

Proof. Let $\eta := (y, y', \dots, y^{(n-1)})$, then $[xy](t) = B(t)\xi(t) \cdot \eta(t)$ by (2.8).

Suppose $U^+x = 0$ is adjoint to $Ux = 0$. By definition of adjoint boundary condition (2.15), U^+ is determined as in Theorem 2.14. But by Theorem 2.14, in determining U^+, there exist boundary forms U_c, U_c^+ of rank $2n - m$ and m, respectively, such that (2.12) holds.

Put

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

Then by the boundary-form formula (2.12),

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

By (2.11),

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

Thus,

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

Thus, we have

$$P_c M + P M_c = -B(a) \qquad\qquad P_c N + P N_c = 0_n$$
$$Q_c M + Q M_c = 0_n \qquad\qquad Q_c N + Q N_c = B(b).$$

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 2.10). 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 (2.17).

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

$$MB^{-1}(a)P_1 = NB^{-1}(b)Q_1 \tag{2.18}$$

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holds.

By the fundamental theorem of linear maps [8, p.63], 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 (2.18),

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

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 $\operatorname{rank}(H) = 2n - m$. Therefore, by (2.17), 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 $U_1^+ y = A^* U^+ y = 0$. Since $A^\star$ is nonsingular, $A^{\star^{-1}}$ is also a linear map, and $A^{\star^{-1}} U_1^+ y = U^+ y$. Thus, $U_1^+ y = 0$ implies $U^+ y = A^{\star^{-1}} U_1^+ y = 0$. Therefore, $U^+ y = 0$ if and only if $U_1^+ y = 0$. Since $U^+ y = 0$ is adjoint to $Ux = 0$, $U_1^+ y = 0$ is adjoint to $Ux = 0$. $\qquad \square$

To recapitulate, the boundary-form formula (Theorem 2.14) gives us the existence and construction of adjoint boundary condition, and Theorem 2.19 gives us a way to check whether a proposed adjoint boundary condition is valid. Now, we are ready to propose a construction algorithm.

3 Algorithm

3.1 Constructing the Adjoint of a Homogeneous Boundary Condition

The adjoint boundary condition associated with the adjoint problem relates to that of the original problem in a way that is important to making the Fokas transform pairs work as we would like them to. Thus, the first step in implementing the Fokas method is to construct the adjoint of a homogeneous boundary condition.

To this end, an algorithm to construct adjoint boundary conditions has been devised and implemented in Julia.

3.2 Constructing the Fokas Transform Pair

3.2.1 Approximating the Roots of an Exponential Polynomial on a Bounded Region

4 Implementation

4.1 Platform

4.2 Examples

5 Discussion

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