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

Capstone Thesis for BSc (Honours) in Mathematical, Computational and Statistical Sciences

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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 (IBVPs) for evolution PDEs in the finite interval [1] based on the Fokas transform method [2][3][4][5][6][7]. The implementation is done in Julia, and, among other functionalities such as numeric evaluation and visualization, features symbolic computation.

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).

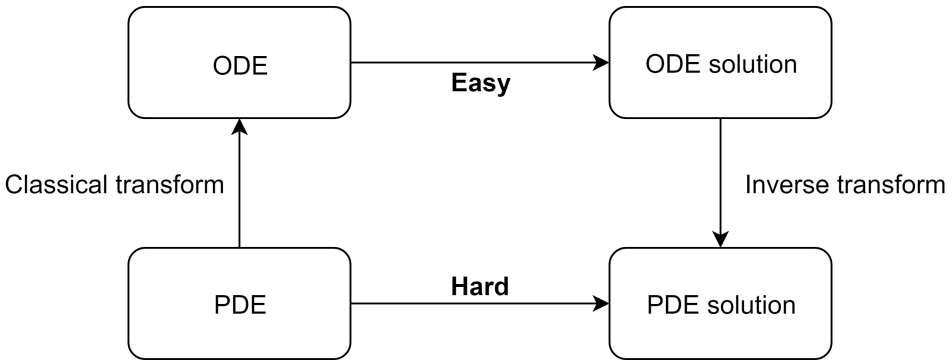


Figure 1: Solving type I IBVPs using classical transform pairs such as the Fourier transform.

For example, the heat equation [8]

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

with periodic boundary conditions

$$\begin{aligned} u(0,t) &= u(L,t), \quad t \in (0,\infty) \\ u_x(0,t) &= u_x(L,t), \quad t \in (0,\infty) \end{aligned}$$

and initial datum

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

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

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

with initial datum

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

where $U(s,t) := \mathcal{F}[u]$ and $F(s) := \mathcal{F}[f]$ are the Fourier transforms of $u(x,t)$ and $f(x)$ with respect to x, respectively.

For more complicated IBVPs (henceforth referred to as type II problems), no such classical transform pairs exist. The linearized Korteweg-de Vries (linearized KdV) equation which describes shallow water waves [9],

$$u_t + u_{xxx} = 0, \tag{1.1}$$

is one such example. 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, as illustrated in Figure 2.

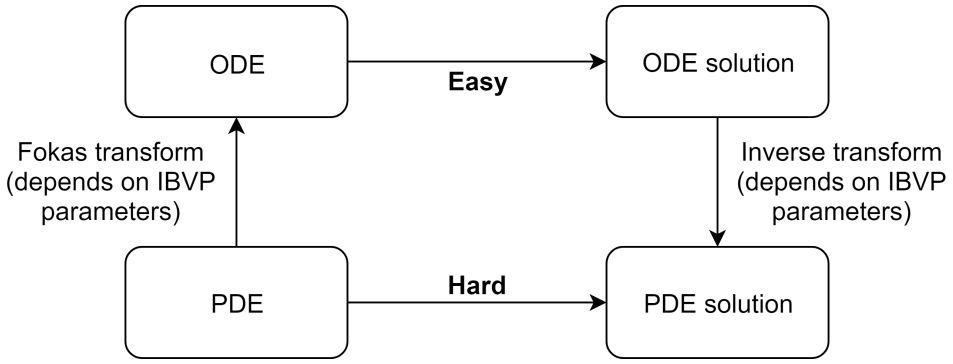


Figure 2: Solving type II IBVPs using the Fokas transform pairs.

Examples of IBVPs that can be solved by the Fokas method include the following IBVPs of the linearized KdV equation [1]:

$$q_t(x,t) + q_{xxx}(x,t) = 0, \qquad (x,t) \in (0,1) \times (0,T) \tag{1.2a}$$
$$q(x,0) = f(x), \qquad x \in [0,1] \tag{1.2b}$$
$$q(0,t) = q(1,t) = 0, \qquad t \in [0,T] \tag{1.2c}$$
$$q_x(1,t) = \frac{1}{2} q_x(0,t) \qquad t \in [0,T], \tag{1.2d}$$

and

$$q_t(x,t) + q_{xxx}(x,t) = 0, \qquad (x,t) \in (0,1) \times (0,T) \tag{1.3a}$$
$$q(x,0) = f(x), \qquad x \in [0,1] \tag{1.3b}$$
$$q(0,t) = q(1,t) = q_x(1,t) = 0, \qquad t \in [0,T]. \tag{1.3c}$$

As will be shown later, the Fokas method is applicable to the more general cases of IBVPs with spatial order n. PDEs of higher order are generally not as well understood as their first and second order counterparts. The Fokas method advances the understanding of higher order PDEs by providing an algorithmic procedure to solve an entire class of IBVPs of arbitrary order. Applying 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. These include visualizations of integration contours, numerical evaluations, and more importantly, derivation of explicit symbolic formulas for important mathematical objects which would help proving technical lemmas that arise in applying the Fokas method to IBVPs [5] and beyond [10].

In this project, the implementation of the Fokas method is developed in Julia, a free open-source, high-performance language for numerical computing [11]. Among tools for numerical computing, commercial software packages 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. At the start of the project, the latest version of Julia is 1.0; however, existing graphing packages in Julia were not yet made compatible with Julia 1.0 at that time. Thus, the project uses the next latest release of Julia that is stable at that time, namely Julia 0.6.4.

To our knowledge, despite the presence of various differential equation solvers in mathematical software such as Julia, Mathematica, and Matlab, this is the first time that the Fokas method is implemented computationally in any generality, and it 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

$$B_j\phi := \sum_{k=0}^{n-1} \left(b_{jk}\phi^{(k)}(0) + \beta_{jk}\phi^{(k)}(1) \right), \; j \in \{1,2,\ldots,n\} \tag{1.4}$$

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

Define the set of smooth functions ϕ that satisfy the homogeneous boundary conditions $B_j\phi = 0$ for $j \in \{1,2,\ldots,n\}$ as

$$\Phi := \{\phi \in C^\infty[0,1] : \; B_j\phi = 0 \, \forall j \in \{1,2,\ldots,n\}\}. \tag{1.5}$$

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

$$S := (-i)^n \frac{d^n}{dx^n}. \tag{1.6}$$

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

$$(\partial_t + aS)q(x,t) = 0 \qquad \forall (x,t) \in (0,1) \times (0,T) \tag{1.7a}$$

$$q(x,0) = f(x) \in \Phi \qquad \forall x \in [0,1] \tag{1.7b}$$

$$q(\cdot,t) \in \Phi \qquad \forall t \in [0,T], \tag{1.7c}$$

where a is a complex constant. For the IBVP to be well-posed, we require at least that $a = \pm i$ if n is odd and $\mathrm{Re}(a) \geq 0$ if n is even. Equation (1.7a) is a PDE in two variables

(spatial variable x and temporal variable t) with arbitrary spatial order n. Equation (1.7b) is an initial datum where the temporal variable $t = 0$. Equation (1.7c) corresponds to the homogeneous spatial boundary conditions, specifying that for any fixed $t \in [0, T]$, $q(x, t) =: \phi(x)$ as a function of x satisfies $B_j\phi = 0$ for $j \in \{1, 2, \ldots, n\}$.

The linearized KdV equations introduced in equation (1.1) are examples of such IBVPs. Specifically, IBVP (1.2) can be written in the form of (1.7) with $a = -i$,

$$S = (-i)^3 \frac{d^3}{dx^3} = i\frac{d^3}{dx^3},$$

$$\begin{aligned}
B_1\phi &= 1 \cdot \phi(0) + 0 \cdot \phi(1) + 0 \cdot \phi^{(1)}(0) + 0 \cdot \phi^{(1)}(1) + 0 \cdot \phi^{(2)}(0) + 0 \cdot \phi^{(2)}(1) \\
B_2\phi &= 0 \cdot \phi(0) + 1 \cdot \phi(1) + 0 \cdot \phi^{(1)}(0) + 0 \cdot \phi^{(1)}(1) + 0 \cdot \phi^{(2)}(0) + 0 \cdot \phi^{(2)}(1) \\
B_3\phi &= 0 \cdot \phi(0) + 0 \cdot \phi(1) + 1 \cdot \phi^{(1)}(0) - 2 \cdot \phi^{(1)}(1) + 0 \cdot \phi^{(2)}(0) + 0 \cdot \phi^{(2)}(1),
\end{aligned}$$

and

$$\Phi = \{\phi \in C^\infty[0, 1] : B_j\phi = 0 \, \forall j \in \{1, 2, 3\}\}.$$

Similarly, IBVP (1.3) can be written in the form of (1.7) with $a = -i$,

$$S = (-i)^3 \frac{d^3}{dx^3} = i\frac{d^3}{dx^3},$$

$$\begin{aligned}
B_1\phi &= 1 \cdot \phi(0) + 0 \cdot \phi(1) + 0 \cdot \phi^{(1)}(0) + 0 \cdot \phi^{(1)}(1) + 0 \cdot \phi^{(2)}(0) + 0 \cdot \phi^{(2)}(1) \\
B_2\phi &= 0 \cdot \phi(0) + 1 \cdot \phi(1) + 0 \cdot \phi^{(1)}(0) + 0 \cdot \phi^{(1)}(1) + 0 \cdot \phi^{(2)}(0) + 0 \cdot \phi^{(2)}(1) \\
B_3\phi &= 0 \cdot \phi(0) + 0 \cdot \phi(1) + 1 \cdot \phi^{(1)}(0) - +0 \cdot \phi^{(1)}(1) + 0 \cdot \phi^{(2)}(0) + 0 \cdot \phi^{(2)}(1),
\end{aligned}$$

and

$$\Phi = \{\phi \in C^\infty[0, 1] : B_j\phi = 0 \, \forall j \in \{1, 2, 3\}\}.$$

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]

$$q(x, t) = f_x(e^{-a\lambda^n t} F_\lambda(f)), \tag{1.8}$$

thus completing the procedure summarised in Figure 2.

2 Preliminaries

We now begin to introduce the preliminary definitions and results used in the algorithmic procedure that finds (1.8). The key to the algorithm is the construction of the Fokas transform pair, which in turn depends on finding a valid adjoint of the given boundary conditions. Thus, we devote the following sections to characterizing the adjoint, and by doing so, outline its construction. These sections present material from chapter 11 of [12], with proofs expanded and completed, and the utility of the theorems expounded.

2.1 Homogeneous boundary value problems

Definition 2.1. [12, 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. [12, 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. [12, 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 [13, p.204]. There exists a similar notion for boundary value problems, which we begin to formulate below.

2.2.1 Adjoint differential operator

Definition 2.4. [12, 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 a set of (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 and their construction.

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

We begin with Green's formula.

Green's formula

Theorem 2.5. *[12, 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 $a \le t_1 < t_2 \le b$ 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

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

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

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

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, for the terms $u^{(k-1)}(t)\bar{v}^{(j-1)}(t)$ with $j+k > n+1$ do 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.

Definition 2.6. [12, p.285] For vectors $f = (f_1, \ldots, f_k)$ and $g = (g_1, \ldots, g_k)$, define the product

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

Note that $f \cdot g = g^* \cdot f$ where * denotes the conjugate transpose.

Definition 2.7. [12, 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

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

then $Sf \cdot g$ is given by

$$\begin{aligned} \mathcal{S}(f,g) := Sf \cdot g &= \begin{bmatrix} s_{11} & \cdots & s_{1k} \\ \vdots & \ddots & \vdots \\ s_{k1} & \cdots & s_{kk} \end{bmatrix} \begin{bmatrix} f_1 \\ \vdots \\ f_k \end{bmatrix} \cdot \begin{bmatrix} g_1 \\ \vdots \\ g_k \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{k} s_{1j} f_j \\ \vdots \\ \sum_{j=1}^{k} s_{kj} f_j \end{bmatrix} \cdot \begin{bmatrix} g_1 \\ \vdots \\ g_k \end{bmatrix} \\ &= \sum_{i=1}^{k} \left(\sum_{j=1}^{k} s_{ij} f_j \right) \bar{g}_i = \sum_{i,j=1}^{k} s_{ij} f_i \bar{g}_i. \end{aligned} \tag{2.7}$$

To see that this is a semibilinear form:

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

and 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 $\vec{u}=(u,u',\dots,u^{(n-1)})$ and $\vec{v}=(v,v',\dots,v^{(n-1)})$. Then we have

$$\begin{aligned}[uv](t)&=\sum_{j,k=1}^{n}B_{jk}(t)u^{(k-1)}(t)\bar{v}^{(j-1)}(t)\quad\text{(by equation (2.5))}\\&=\sum_{i,j=1}^{n}(B_{ij}u^{(j-1)}\overline{v}^{(i-1)})(t)\\&=(B\vec{u}\cdot\vec{v})(t)\quad\text{(by equation (2.7))}\\&=:\mathcal{S}(\vec{u},\vec{v})(t).\end{aligned}\tag{2.8}$$

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 & \ddots & \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 & \ddots & \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 & \ddots & \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 & \ddots & \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 & \ddots & \vdots & \vdots & \ddots & \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 & \ddots & \vdots & \vdots & \ddots & \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{2.9}
$$

Recall that $\det(\lambda A) = \lambda^n \det(A)$ for $n \times n$ matrix A. Thus, since $B(t_1)$ is $n \times n$, we have

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

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 defined on an interval $[a, b]$ with coefficients $p_0(t), \dots, p_n(t)$, from the Green's formula, we have defined a matrix B which depends on $p_0, \dots, p_n$ 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 the following definitions and results concerning boundary conditions.

Definition 2.8. [12, 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. [12, p.286] A **vector boundary form** $U = (U_1, \ldots, U_m)$ is a vector whose components are boundary forms. When $U_1, \ldots, U_m$ are linearly independent, we say that U has full rank m. We assume U has full rank below.

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

$$\xi := \begin{bmatrix} x & x^{(1)} & \cdots & x^{(n-1)} \end{bmatrix}^{\intercal}, \tag{2.11}$$

$$U := \begin{bmatrix} U_1 & U_2 & \cdots & U_m \end{bmatrix}^{\intercal}, \tag{2.12}$$

and

$$M := \begin{bmatrix} M_{11} & \cdots & M_{1n} \\ \vdots & \ddots & \vdots \\ M_{m1} & \cdots & M_{mn} \end{bmatrix}, \quad N := \begin{bmatrix} N_{11} & \cdots & N_{1n} \\ \vdots & \ddots & \vdots \\ N_{m1} & \cdots & N_{mn} \end{bmatrix}. \tag{2.13}$$

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

$$Ux = M\xi(a) + N\xi(b). \tag{2.14}$$

Indeed:

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

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

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

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

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

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

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. [12, p.287] If $U = (U_1, \ldots, U_m)$ is any boundary form with $\operatorname{rank}(U) = m$ and $U_c = (U_{m+1}, \ldots, U_{2n})$ is any form with $\operatorname{rank}(U_c) = 2n - m$ 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. *[12, p.287] In the context of the semibilinear form* (2.7)*, we have*

$$Sf \cdot g = f \cdot S^* g, \tag{2.15}$$

where * denotes the conjugate transpose.

Proof.

$$
\begin{aligned}
Sf \cdot g &= \sum_{i,j=1}^{k} s_{ij} f_j \bar{g}_i \quad \text{(by equation (2.7))};\\
f \cdot S^* g &= \begin{bmatrix} f_1 \\ \vdots \\ f_k \end{bmatrix} \cdot \begin{bmatrix} \bar{s}_{11} & \cdots & \bar{s}_{k1} \\ \vdots & \ddots & \vdots \\ \bar{s}_{1k} & \cdots & \bar{s}_{kk} \end{bmatrix} \begin{bmatrix} g_1 \\ \vdots \\ g_k \end{bmatrix} \\
&= \begin{bmatrix} f_1 \\ \vdots \\ f_k \end{bmatrix} \cdot \begin{bmatrix} \sum_{j=1}^{k} \bar{s}_{j1} g_j \\ \vdots \\ \sum_{j=1}^{k} \bar{s}_{jk} g_j \end{bmatrix} \\
&= \sum_{i=1}^{k} f_i \cdot \overline{\left(\sum_{j=1}^{k} \bar{s}_{ji} g_j \right)} \\
&= \sum_{i=1}^{k} f_i \cdot \left(\sum_{j=1}^{k} s_{ji} \bar{g}_j \right) \\
&= \sum_{i,j=1}^{k} s_{ji} f_i \bar{g}_j = Sf \cdot g. \qquad \square
\end{aligned}
$$

Proposition 2.12. *[12, 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

$$
\begin{aligned}
\mathcal{S}(f, g) &= Sf \cdot g \\
&= S(F^{-1}F) f \cdot g \\
&= SF^{-1}(Ff) \cdot g \\
&= SF^{-1} \bar{f} \cdot g \\
&= \bar{f} \cdot (SF^{-1})^* g \quad \text{(by equation (2.15))} \\
&= \bar{f} \cdot G * g \\
&= \bar{f} \cdot \bar{g}.
\end{aligned}
$$

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. $\square$

Proposition 2.13. *[12, 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,

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

(where the third equality follows from a reverse application of equation (2.15) 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 conditions.

Theorem 2.14. *[12, p.288](Boundary-form formula) Given any boundary form U of rank m, and any complementary form U_c, there exist unique boundary forms U_c^+, U^+ of rank m and $2n-m$, respectively, such that*

$$[xy](b) - [xy](a) = Ux \cdot U_c^+ y + U_c x \cdot U^+ y. \tag{2.16}$$

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

$$\tilde{U}^+ y = C^* U^+ y \tag{2.17}$$

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 equation (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 equation (2.9) that the left-hand side of equation (2.16) 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 equation (2.6). Recall from equation (2.14) that

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

for ξ, M, N defined in equation (2.11) and equation (2.13). 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 $G = (SF^{-1})^*$, we have $J = (\hat{B}H^{-1})^*$) 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, equation (2.16) holds.

The second statement in the theorem follows from Proposition 2.13 with Hf and Jg corresponding to f and g. □

Characterization of adjoint boundary conditions

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 their construction.

Definition 2.16. [12, p.288-89] For any boundary form U of rank m there is associated the homogeneous boundary condition

$$Ux = 0 \tag{2.18}$$

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

$$U^+ x = 0 \tag{2.19}$$

is an **adjoint boundary condition** to (2.18).

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

Definition 2.17. [12, 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 equation (2.2).

Proposition 2.18. *By Green's formula* (2.3) *and the boundary-form formula* (2.16)*,*

$$\langle Lu, v \rangle = \langle u, L^+ v \rangle$$

for all $u \in C^n$ *on* $[a,b]$ *satisfying equation* (2.18) *and all* $v \in C^n$ *on* $[a,b]$ *satisfying equation* (2.19)*.*

Proof.

$$\begin{aligned}\langle Lu, v\rangle - \langle u, L^+v\rangle &= \int_a^b Lu\bar{v}\,dt - \int_a^b u(\overline{L^+v})\,dt \\ &= [uv](a) - [uv](b) \quad \text{(by Green's formula (2.3))} \\ &= Uu \cdot U_c^+ v + U_c u \cdot U^+ v \quad \text{(by boundary-form formula (2.16))} \\ &= 0 \cdot U_c^+ v + U_c u \cdot 0 \quad \text{(by equation (2.18) and equation (2.19))} \\ &= 0.\end{aligned}$$

□

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 adjoint problem is introduced using linear algebra, as described in the introduction to section 2.2. 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

$$U^+x = P^*\xi(a) + Q^*\xi(b). \tag{2.20}$$

The following theorem is motivated by characterizing the homogeneous boundary condition and its adjoint ((2.19) – (2.18)) in terms of the matrices M, N, P, Q. For our purpose, it provides a means to check whether the adjoint boundary condition we found via the boundary-form formula (Theorem 2.14) is indeed valid.

Theorem 2.19. *[12, p.289] The boundary condition $U^+x = 0$ is adjoint to $Ux = 0$ if and only if*

$$MB^{-1}(a)P = NB^{-1}(b)Q \tag{2.21}$$

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

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

Suppose $U^+x = 0$ is adjoint to $Ux = 0$. By definition of adjoint boundary condition (2.19), 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 equation (2.16) 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 (2.16),

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

By equation (2.15),

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

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

$$\begin{aligned} P_cM + PM_c &= -B(a) & P_cN + PN_c &= 0_n \\ Q_cM + QM_c &= 0_n & Q_cN + QN_c &= B(b). \end{aligned}$$

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. 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 equation (2.21).

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

$$MB^{-1}(a)P_1 = NB^{-1}(b)Q_1 \tag{2.22}$$

holds.

By the fundamental theorem of linear maps [13, 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 equation (2.22),

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

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 equation (2.21), 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 $U_1^+y = A^*U^+y = 0$. Since A^* is nonsingular, $A^{*^{-1}}$ is also a linear map, and $A^{*^{-1}}U_1^+y = U^+y$. Thus, $U_1^+y = 0$ implies $U^+y = A^{*^{-1}}U_1^+y = 0$. 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 $Ux = 0$. □

To recapitulate, the boundary-form formula (Theorem 2.14) provides the existence and construction of adjoint boundary condition, and Theorem 2.19 supplies a means to check whether a proposed adjoint boundary condition is valid. With these results, we are ready to formulate an algorithmic procedure to solve (1.7) using the Fokas method.

3 Algorithm

Consider an IBVP of the form (1.7). We now outline the algorithm to find its solution. The solution is given in equation (3.8), via explicit construction of an integral transform and inverse transform pair. In this section, we provide that explicit mathematical construction, and adapt it into an algorithm that can be implemented in software. The transform pair is displayed in equation (3.7), using notations developed throughout section 3.2.

3.1 Constructing the adjoint of a set of homogeneous boundary conditions

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. In fact, the first step in implementing the Fokas method is to construct the adjoint of a set of homogeneous boundary conditions. To this end, an algorithm to construct adjoint boundary conditions has been devised and implemented in Julia, outlined as follows.

Define the differential operator

$$L := S$$

to be the spatial differential operator in equation (1.6), the interval

$$[a, b] := [0, 1]$$

to be the unit interval in (1.7), and U to be the vector boundary form associated with two $n \times n$ matrices M, N given entry-wise by

$$M_{jk} := b_{jk}, \quad N_{jk} := \beta_{jk}$$

for b_{jk}, β_{jk} in equation (1.4). Then we have defined a boundary-value problem in the spatial variable from the original IBVP, namely

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

We seek to construct a valid adjoint boundary condition $U^+x = 0$.

3.1.1 Checking input

We first check that $U_1, \ldots, U_n$ are linearly independent. Recall from equation (2.14) that

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

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

3.1.2 Finding a candidate adjoint

Recall from Definition 2.10 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 embedding $(M : N)$ in a $2n \times 2n$ nonsingular matrix (where the newly added rows constitute $(\tilde{M}, \tilde{N})$ associated with U_c). Thus, we can construct this $2n \times 2n$ nonsingular matrix as follows: Given the identity matrix E_{2n} and the $n \times 2n$ matrix $(M : N)$, we append the rows of E_{2n} one by one to $(M : N)$ and retain only those rows that make the rank of the resulting matrix increase.

The output from the above construction is a $2n \times 2n$ matrix of the form

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

where the rows of 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 2.14 (where $\tilde{M}, \tilde{N}$ are associated with the complementary boundary form $U_c x = \tilde{M}\xi(a) + \tilde{N}\xi(b)$).

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 (2.6) which depends on $p_0, \ldots, p_n$. Construct $\hat{B}$ from B and $[a, b]$ as in Theorem 2.14. Let $J := (\hat{B}H^{-1})^*$. By Theorem 2.14 and Proposition 2.12, the matrix J is of the form

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

where $\tilde{M}', \tilde{N}'$ are associated with an adjoint U^+ and M', N' with its complement U_c^+. Thus, we can identify $(P^* : Q^*)$ with the last n rows of J. That is, identify P^* with $\tilde{M}'$, the lower-left $n \times n$ submatrix of J, and Q^* with $\tilde{N}'$, the lower-right $n \times n$ submatrix of J. Define U^+ by

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

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

3.1.3 Checking the validity of the candidate adjoint

By Theorem 2.19, with

$$Ux = M\xi(a) + N\xi(b), \quad U^+ x = P^*\xi(a) + Q^*\xi(b) \tag{3.1}$$

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 (2.6).

It may be worth noting that although the spatial differential operator which the above procedure will be applied to when using the Fokas method assumes the specific form given by equation (1.6), the procedure in fact works for any general linear differential operator. Systematic unit tests have been developed [16] to test the procedure's implementation in Julia, accounting for linear differential operators with constant coefficients and polynomial coefficients.

3.2 Constructing the Fokas transform pair

This section presents materials from [1], with definitions expanded and adapted to the algorithm.

Define the matrices

$$b^\star := P^*, \quad \beta^\star := Q^*,$$

where P^*, Q^* are the matrices associated with the adjoint vector boundary form U^+ in equation 3.1. Let $\alpha := e^{2\pi i/n}$. For complex variable λ, define $W^+(\lambda)$, $W^-(\lambda)$ as the $n \times n$ matrices whose kj-entries are given by

$$W_{kj}^+(\lambda) := \sum_{r=0}^{n-1} (-i\alpha^{k-1}\lambda)^r b_{jr}^\star \tag{3.2a}$$

$$W_{kj}^-(\lambda) := \sum_{r=0}^{n-1} (-i\alpha^{k-1}\lambda)^r \beta_{jr}^\star, \tag{3.2b}$$

where $b^\star_{jr}$, $\beta^\star_{jr}$ are indexed from 0 to $n-1$ in r. Define W as the $n \times n$ matrix whose kj-entry is given by

$$W_{kj}(\lambda) := W^+_{kj}(\lambda) + W^-_{kj}(\lambda) e^{-\alpha^{k-1}\lambda}. \tag{3.3}$$

Let

$$\Delta(\lambda) := \det W(\lambda). \tag{3.4}$$

Note that by the definition of $W(\lambda)$, Δ is an exponential polynomial in λ. That is,

$$\Delta(\lambda) = \sum_{k=1}^{m} a_k \lambda^k e^{b_k \lambda},$$

where $a_k, b_k \in \mathbb{C}$ for $k \in \{1, \dots, m\}$.

Let X^{lj} be the $(n-1) \times (n-1)$ submatrix of the block matrix $\mathbb{W} := \begin{bmatrix} W & W \\ W & W \end{bmatrix}$, where X^{lj}_{11} is $\mathbb{W}_{l+1,j+1}$.

For $\lambda \in \mathbb{C}$ such that $\Delta(\lambda) \neq 0$, define

$$F^+_\lambda(f) := \frac{1}{2\pi\Delta(\lambda)} \sum_{l=1}^{n} \sum_{j=1}^{n} (-1)^{(n-1)(l+j)} \det X^{lj}(\lambda) W^+_{1j}(\lambda) \int_0^1 e^{-i\alpha^{l-1}\lambda x} f(x)\, dx \tag{3.5a}$$

$$F^-_\lambda(f) := \frac{-e^{-i\lambda}}{2\pi\Delta(\lambda)} \sum_{l=1}^{n} \sum_{j=1}^{n} (-1)^{(n-1)(l+j)} \det X^{lj}(\lambda) W^-_{1j}(\lambda) \int_0^1 e^{-i\alpha^{l-1}\lambda x} f(x)\, dx. \tag{3.5b}$$

By the theory of exponential polynomials [14], the infimum of the distances between every two distinct zeros of $\Delta(\lambda)$ is positive. Let 5ϵ be such this infimum. Let ∂S denote boundary of set S. Let $\operatorname{cl} S$ denote the closure of set S. Let $\mathbb{C}^\pm$ denote the open upper and open lower halves of the complex plane, respectively. Let $D(x_0, \epsilon)$ denote the disk $\{x \in \mathbb{C} : |x - x_0| < \epsilon\}$ centered at x_0 with radius ϵ. Let $C(x_0, \epsilon)$ denote the circle $\{x \in \mathbb{C} : |x - x_0| = \epsilon\}$ centered at x_0 with radius ϵ. Define the contours

$$\Gamma^\pm_a := \partial \left(\{\lambda \in \mathbb{C}^\pm : \operatorname{Re}(a\lambda^n) > 0\} \setminus \bigcup_{\substack{\sigma \in \mathbb{C}; \\ \Delta(\sigma)=0}} D(\sigma, 2\epsilon) \right) \tag{3.6a}$$

$$\Gamma_a := \Gamma^+_a \cup \Gamma^-_a \tag{3.6b}$$

$$\Gamma^+_0 := \bigcup_{\substack{\sigma \in \operatorname{cl} \mathbb{C}^+; \\ \Delta(\sigma)=0}} C(\sigma, \epsilon) \tag{3.6c}$$

$$\Gamma^-_0 := \bigcup_{\substack{\sigma \in \mathbb{C}^-; \\ \Delta(\sigma)=0}} C(\sigma, \epsilon) \tag{3.6d}$$

$$\Gamma_0 := \Gamma^+_0 \cup \Gamma^-_0 \tag{3.6e}$$

$$\Gamma := \Gamma_0 \cup \Gamma_a. \tag{3.6f}$$

A sample contour is shown in Figure 3.

The Fokas transform pair is given by

$$F_\lambda : f(x) \mapsto F(\lambda) \quad F_\lambda(f) = \begin{cases} F^+_\lambda(f) & \text{if } \lambda \in \Gamma^+_0 \cup \Gamma^+_a, \\ F^-_\lambda(f) & \text{if } \lambda \in \Gamma^-_0 \cup \Gamma^-_a, \end{cases} \tag{3.7a}$$

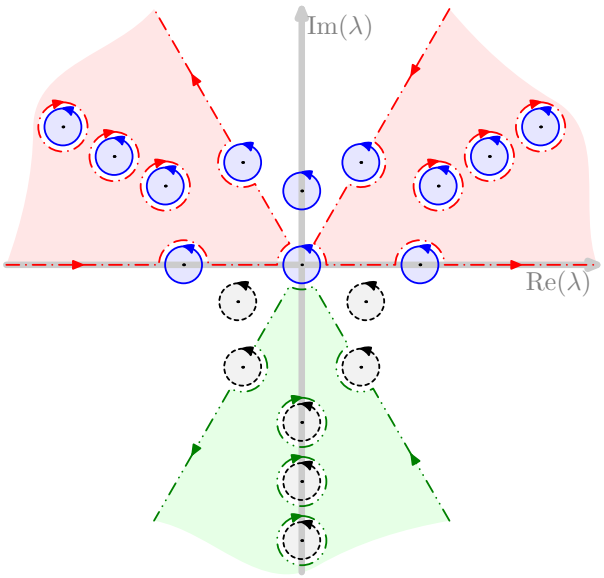


Figure 3: Hypothetical Γ contours corresponding to the case $a = -i$, taken from [1]. The red dashed lines correspond to Γ_a^+, and the green dashed lines correspond to Γ_a^-. The blue circles correspond to Γ_0^+, and the black circles correspond to Γ_0^-. The arrows indicate the order of integration in equation (3.8).

$$f_x : F(\lambda) \mapsto f(x) \quad f_x(F) = \int_\Gamma e^{i\lambda x} F(\lambda)\, d\lambda,\ x \in [0,1], \tag{3.7b}$$

which allows computing the IBVP solution $q(x,t)$ in (1.8) by

$$\begin{aligned} q(x,t) &= f_x\left(e^{-a\lambda^n t} F_\lambda(f)\right) \\ &= \int_{\Gamma_0^+} e^{i\lambda x} e^{-a\lambda^n t} F_\lambda^+(f)\, d\lambda + \int_{\Gamma_a^+} e^{i\lambda x} e^{-a\lambda^n t} F_\lambda^+(f)\, d\lambda \\ &\quad + \int_{\Gamma_0^-} e^{i\lambda x} e^{-a\lambda^n t} F_\lambda^-(f)\, d\lambda + \int_{\Gamma_a^-} e^{i\lambda x} e^{-a\lambda^n t} F_\lambda^-(f)\, d\lambda. \end{aligned} \tag{3.8}$$

As shown above in (3.7), the Fokas transform pair is a pair of contour integral transform and inverse transform. Thus, to construct the transform pair, we need to construct the integrands F_λ^+. F_λ^-, and the contours Γ over which the integrands are to be integrated.

3.2.1 Constructing the integrands

Theoretically, the integrands F_λ^+ and F_λ^- can be computed directly from (3.5). Yet there is a complication in practice. As shown in equation (3.8), the definition of the solution $q(x,t)$ involves integrals of F_λ^+, F_λ^- over the contours Γ, but as shown in (3.5a)–(3.5b), F_λ^+ and F_λ^- themselves involve an integral of the initial datum $f(x)$. Double integrals are computationally expensive, and so to improve algorithm efficiency, we replace the inner integral involving $f(x)$ with an approximation of it that has explicit formula, developed as follows.

Approximating inner integral using Chebyshev polynomials

The inner integral we wish to compute is

$$\int_0^1 e^{-i\alpha^{l-1}\lambda x} f(x)\, dx.$$

Note that this is the Fourier transform of f defined on $[0,1]$ evaluated at $\alpha^{l-1}\lambda$. The idea is to approximate $f(x)$ using Chebyshev polynomials and compute the integral using explicit formula of the Fourier Transform of Chebyshev polynomials [15].

The Chebyshev polynomials are given by

$$T_n(x) = \begin{cases} \cos(n \arccos(x)) & |x| \leq 1 \\ \frac{1}{2}\left((x - \sqrt{x^2-1})^n + (x + \sqrt{x^2-1})^n\right) & |x| > 1. \end{cases}$$

Given a function f on the interval $[a,b]$, we can approximate f using Chebyshev polynomial expansion. The Chebyshev approximation is best on $[-1,1]$. Thus, we scale $[a,b]$ to $[-1,1]$ via $g : [a,b] \to [-1,1]$ given by $g(x) = 2(x-a)/(b-a) - 1$, obtain the Chebyshev coefficients $\{b_n\}_{n=0}^N$ there, and write the approximation of f on $[a,b]$ as

$$f \approx \sum_{n=0}^{N} b_n \cdot T_n(g(x)),$$

which is a finite sum of Chebyshev polynomials.

Now, suppose we are given the IBVP's initial datum $f(x)$. Define $g(x) : [0,1] \to [-1,1]$ by $g(x) = 2x - 1$. With the change of variable $t = g(x) = 2x - 1$, we have $x = g^{-1}(t) = \frac{t+1}{2}$. Writing $c = \frac{\alpha^{l-1}\lambda}{2}$, we have

$$\begin{aligned} \int_0^1 e^{-i\alpha^{l-1}\lambda x} f(x)\, dx &= \int_0^1 e^{-i2c\frac{t+1}{2}} f\left(\frac{t+1}{2}\right)\, d\left(\frac{t+1}{2}\right) \\ &= \int_{-1}^1 e^{-ict} e^{-ic} f\left(\frac{t+1}{2}\right) \frac{1}{2}\, dt \\ &= \frac{1}{2e^{ic}} \int_{-1}^1 e^{-ict} f\left(\frac{t+1}{2}\right)\, dt \\ &= \frac{1}{2e^{ic}} \int_{-1}^1 e^{-ict} q(t)\, dt, \end{aligned}$$

where $q(t) := f \circ g^{-1}(t)$. Thus, it suffices to find

$$\int_{-1}^1 e^{-ict} q(t)\, dt.$$

Suppose that on $[-1,1]$,

$$q(t) \approx \sum_{n=0}^{N} b_n T_n(t).$$

(Note that since $t = g(x)$, the Chebyshev coefficients of q are exactly the coefficients of f obtained on $[-1,1]$.) Then since $t \in [-1,1]$,

$$q(t) \approx \sum_{n=0}^{N} b_n \cos(n \arccos(t)),$$

and so

$$\int_{-1}^1 e^{-ict} q(t)\, dt = \int_{-1}^1 e^{-ict} \sum_{n=0}^{N} b_n \cos(n \arccos(t))\, dt$$

$$= \sum_{n=0}^{N} b_n \int_{-1}^{1} e^{-ict} \cos(n \arccos(t))\, dt.$$

With the change of variable $t = \cos\theta$,

$$\begin{aligned}\int_{-1}^{1} e^{-ict} \cos(n \arccos(t))\, dt &= \int_{-1}^{1} e^{-ic\cos\theta} \cos(n \arccos(\cos\theta))\, d\cos\theta \\ &= \int_{\pi}^{0} e^{-ic\cos\theta} \cos(n\theta)(-\sin\theta)\, d\theta \\ &= \int_{0}^{\pi} e^{-ic\cos\theta} \cos(n\theta)\sin\theta\, d\theta.\end{aligned}$$

Define

$$\tilde{T}_n(c) := \int_{0}^{\pi} e^{-ic\cos\theta} \cos(n\theta)\sin\theta\, d\theta.$$

Then

$$\begin{aligned}\tilde{T}_n(0) = \int_{0}^{\pi} \cos(n\theta)\sin\theta\, d\theta &= \begin{cases} 2 & \text{if } n = 0 \\ [\frac{1}{2}\sin^2\theta + \frac{0}{2}\cos^2\theta]_0^{\pi} & \text{if } n = 1 \\ \left[\frac{n}{(n-1)(n+1)}\sin\theta\sin(n\theta) + \frac{1}{(n-1)(n+1)}\cos\theta\cos(n\theta)\right]_0^{\pi} & \text{if } n \geq 2 \end{cases} \\ &= \begin{cases} 2 & \text{if } n = 0 \\ \frac{1}{2}\sin^2(\pi) - \frac{1}{2}\sin^2(0) & \text{if } n = 1 \\ \frac{n}{n^2-1}\sin(\pi)\sin(n\pi) + \frac{1}{n^2-1}\cos(\pi)\cos(n\pi) & \\ \qquad -\frac{n}{n^2-1}\sin(0)\sin(0) - \frac{1}{n^2-1}\cos(0)\cos(0) & \text{if } n \geq 2 \end{cases} \\ &= \begin{cases} 2 & \text{if } n = 0 \\ 0 & \text{if } n = 1 \\ \frac{(-1)^{n+1}-1}{n^2-1} & \text{if } n \geq 2 \end{cases}.\end{aligned}$$

For $c \in \mathbb{C} \setminus \{0\}$, using integration by parts,

$$\begin{aligned}\tilde{T}_n(c) &= \int_{0}^{\pi} e^{-ic\cos\theta} \cos(n\theta)\sin\theta\, d\theta \\ &= \left[\cos(n\theta)\frac{1}{ic}e^{-ic\cos\theta}\right]_0^{\pi} - \int_{0}^{\pi} \frac{1}{ic}e^{-ic\cos\theta} n(-\sin(n\theta))\, d\theta \\ &= \left[\cos(n\pi)\frac{1}{ic}e^{-ic\cos(\pi)} - \cos(0)\frac{1}{ic}e^{-ic\cos 0}\right] + \frac{n}{ic}\int_{0}^{\pi} e^{-ic\cos\theta}\sin(n\theta)\, d\theta \\ &= \frac{1}{ic}\left(n\int_{0}^{\pi} e^{-ic\cos\theta}\sin(n\theta)\, d\theta + (-1)^n e^{ic} - e^{-ic}\right).\end{aligned}$$

Let $z \in \mathbb{C} \setminus \{0\}$, define

$$K_n(z) := \int_{0}^{\pi} e^{z\cos\theta}\sin(n\theta)\, d\theta.$$

Then

$$K_0(z) = \int_{0}^{\pi} e^{z\cos\theta}\sin 0\, d\theta = 0,$$

$$\begin{aligned} K_1(z) &= \int_0^\pi e^{z\cos\theta}\sin\theta\,d\theta \\ &= \left[-\frac{1}{z}e^{z\cos\theta}\right]_0^\pi \\ &= -\frac{1}{z}e^{z\cos(\pi)} + \frac{1}{z}e^{z\cos 0} \\ &= \frac{e^z - e^{-z}}{z} \end{aligned}$$

To compute $K_n(z)$ for $n \geq 2$, we first note that

$$\begin{aligned} \sin((n+1)\theta) - \sin((n-1)\theta) &= \frac{e^{i(n+1)\theta} - e^{-i(n+1)\theta}}{2i} - \frac{e^{i(n-1)\theta} - e^{-i(n-1)\theta}}{2i} \\ &= \frac{e^{in\theta}e^{i\theta} - e^{in\theta}e^{-\theta} - e^{-in\theta}e^{-i\theta} + e^{-in\theta}e^{i\theta}}{2i} \\ &= \frac{(e^{i\theta} - e^{-i\theta})(e^{in\theta} + e^{-in\theta})}{2i} \\ &= 2\left(\frac{e^{i\theta} - e^{-i\theta}}{2i}\right)\left(\frac{e^{in\theta} + e^{-in\theta}}{2}\right) \\ &= 2\sin\theta\cos(n\theta). \end{aligned}$$

So

$$\sin((n+1)\theta) = \sin((n-1)\theta) + 2\sin\theta\cos(n\theta).$$

Thus,

$$\begin{aligned} K_{n+1}(z) &= \int_0^\pi e^{z\cos\theta}\sin((n+1)\theta)\,d\theta \\ &= \int_0^\pi e^{z\cos\theta}(\sin((n-1)\theta) + 2\sin\theta\cos(n\theta))\,d\theta \\ &= \int_0^\pi e^{z\cos\theta}\sin((n-1)\theta)\,d\theta + 2\int_0^{\frac{\pi}{2}} e^{z\cos\theta}\sin\theta\cos(n\theta)\,d\theta \\ &= K_{n-1}(z) + 2\int_0^\pi \cos(n\theta)\sin\theta e^{z\cos\theta}\,d\theta. \end{aligned}$$

Using integration by parts,

$$\begin{aligned} \int_0^\pi \cos(n\theta)\sin\theta e^{z\cos\theta}\,d\theta &= \left[-\frac{1}{z}e^{z\cos\theta}\cos(n\theta)\right]_0^\pi - \int_0^\pi \frac{1}{z}e^{z\cos\theta}n\sin(n\theta)\,d\theta \\ &= -\frac{1}{z}e^{z\cos(\pi)}\cos(n\pi) + \frac{1}{z}e^{z\cos 0}\cos 0 - \frac{n}{z}\int_0^\pi e^{z\cos\theta}\sin(n\theta)\,d\theta \\ &= \frac{e^z}{z} + (-1)^{n+1}\frac{e^{-z}}{z} - \frac{n}{z}K_n(z). \end{aligned}$$

Thus, $K_n(z)$ satisfies the recurrence relation

$$\begin{aligned} K_0(z) &= 0 \\ K_1(z) &= \frac{e^z - e^{-z}}{z} \end{aligned}$$

$$K_n(z) = K_{n-2}(z) + 2\left(\frac{e^z}{z} + (-1)^n\frac{e^{-z}}{z} - \frac{n-1}{z}K_{n-1}(z)\right), \quad n \geq 2.$$

Hence, for $c \in \mathbb{C} \setminus \{0\}$,

$$\begin{aligned}\tilde{T}_n(c) &= \frac{1}{ic}\left(n\int_0^\pi e^{-ic\cos\theta}\sin(n\theta)\,d\theta + (-1)^n e^{ic} - e^{-ic}\right)\\ &= \frac{1}{ic}\left(nK_n(-ic) + (-1)^n e^{ic} - e^{-ic}\right).\end{aligned}$$

Further solving the recurrence relation [15] gives

$$\begin{aligned}\tilde{T}_n(c) = \int_0^\pi e^{-ic\cos\theta}\cos(n\theta)\sin\theta\,d\theta &= \begin{cases}2 & \text{if } n=0,\\ 0 & \text{if } n=1,\\ \frac{(-1)^{n+1}-1}{n^2-1} & \text{if } n\geq 2,\end{cases} && \text{if } c=0,\\ &= \sum_{m=1}^{n+1}\alpha(m,n)\left[\frac{e^{i\lambda}}{(i\lambda)^m} + (-1)^{m+n}\frac{e^{-i\lambda}}{(i\lambda)^m}\right] && \text{if } c\neq 0,\end{aligned}$$

where

$$\alpha(m,n) = \begin{cases}(-1)^n & \text{if } m=1,\\ (-1)^{n+1}n^2 & \text{if } m=2,\\ (-1)^{n+m-1}2^{m-2}n\sum_{k=1}^{n-m+2}\binom{m+k-3}{k-1}\prod_{j=k}^{m+k-3}(n-j) & \text{else.}\end{cases}$$

Thus, in summary,

$$\begin{aligned}\int_0^1 e^{-i\alpha^{l-1}\lambda x}f(x)\,dx &= \frac{1}{2e^{ic}}\int_{-1}^1 e^{-ict}q(t)\,dt\\ &= \frac{1}{2e^{ic}}\sum_{n=0}^N b_n\int_{-1}^1 e^{-ict}\cos(n\arccos(t))\,dt\\ &= \frac{1}{2e^{ic}}\sum_{n=0}^N b_n\hat{T}_n(t).\end{aligned}$$

3.2.2 Constructing the contours

We now set out to find an explicit characterization of the contours Γ.

We note that by (3.6), Γ_a^+ and Γ_a^- are boundaries of the region $\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}$ in the upper and lower half planes, respectively, deformed to avoid zeros of $\Delta(\lambda)$. On the other hand, Γ_0^+ and Γ_0^- consist of circles of radius ϵ around zeros of $\Delta(\lambda)$ in the closed upper half plane and the open lower half plane, respectively. Thus, to find Γ, we need to find the region $\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}$ and the zeros of $\Delta(\lambda)$.

Tracing contour backbone

We first find the region

$$\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}.$$

For $z \in \mathbb{C}$, define $\theta_z := \arg(z)$ and $r_z := |z|$. Let $\lambda \in \mathbb{C}$. Then

$$a\lambda^n = r_a e^{i\theta_a}\cdot r_\lambda^n e^{ni\theta_\lambda} = r_a r_\lambda^n e^{i(\theta_a + n\theta_\lambda)} = r_a r_\lambda^n(\cos(\theta_a + n\theta_\lambda) + i\sin(\theta_a + n\theta_\lambda)).$$

Thus,

$$\mathrm{Re}(a\lambda^n) = r_a r_\lambda^n \cos(\theta_a + n\theta_\lambda),$$

where

$$\mathrm{Re}(a\lambda^n) > 0 \iff \cos(\theta_a + n\theta_\lambda) > 0.$$

But

$$\cos(\theta_a + n\theta_\lambda) > 0 \iff \theta_a + n\theta_\lambda \in \bigcup_{k\in\mathbb{Z}} \left(2\pi k - \frac{\pi}{2},\, 2\pi k + \frac{\pi}{2}\right),$$

and so

$$\theta_\lambda \in \bigcup_{k\in\mathbb{Z}} \left(\frac{2\pi k - \frac{\pi}{2} - \theta_a}{n},\, \frac{2\pi k + \frac{\pi}{2} - \theta_a}{n}\right).$$

For example, when $a = -i$ and $n = 3$,

$$\theta_\lambda \in \bigcup_{k\in\mathbb{Z}} \left(\frac{2\pi k - \frac{\pi}{2} - (-\frac{\pi}{2})}{3},\, \frac{2\pi k + \frac{\pi}{2} - (-\frac{\pi}{2})}{3}\right) = \bigcup_{k\in\mathbb{Z}} \left(\frac{2\pi k}{3},\, \frac{2\pi k + \pi}{3}\right).$$

Thus, in $[0, 2\pi)$,

$$\theta_\lambda = \arg(\lambda) \in \bigcup_{k\in\{0,1,2\}} \left(\frac{2\pi k}{3},\, \frac{2\pi k + \pi}{3}\right) = \left(0, \frac{\pi}{3}\right) \cup \left(\frac{2\pi}{3}, \pi\right) \cup \left(\frac{4\pi}{3}, \frac{5\pi}{3}\right).$$

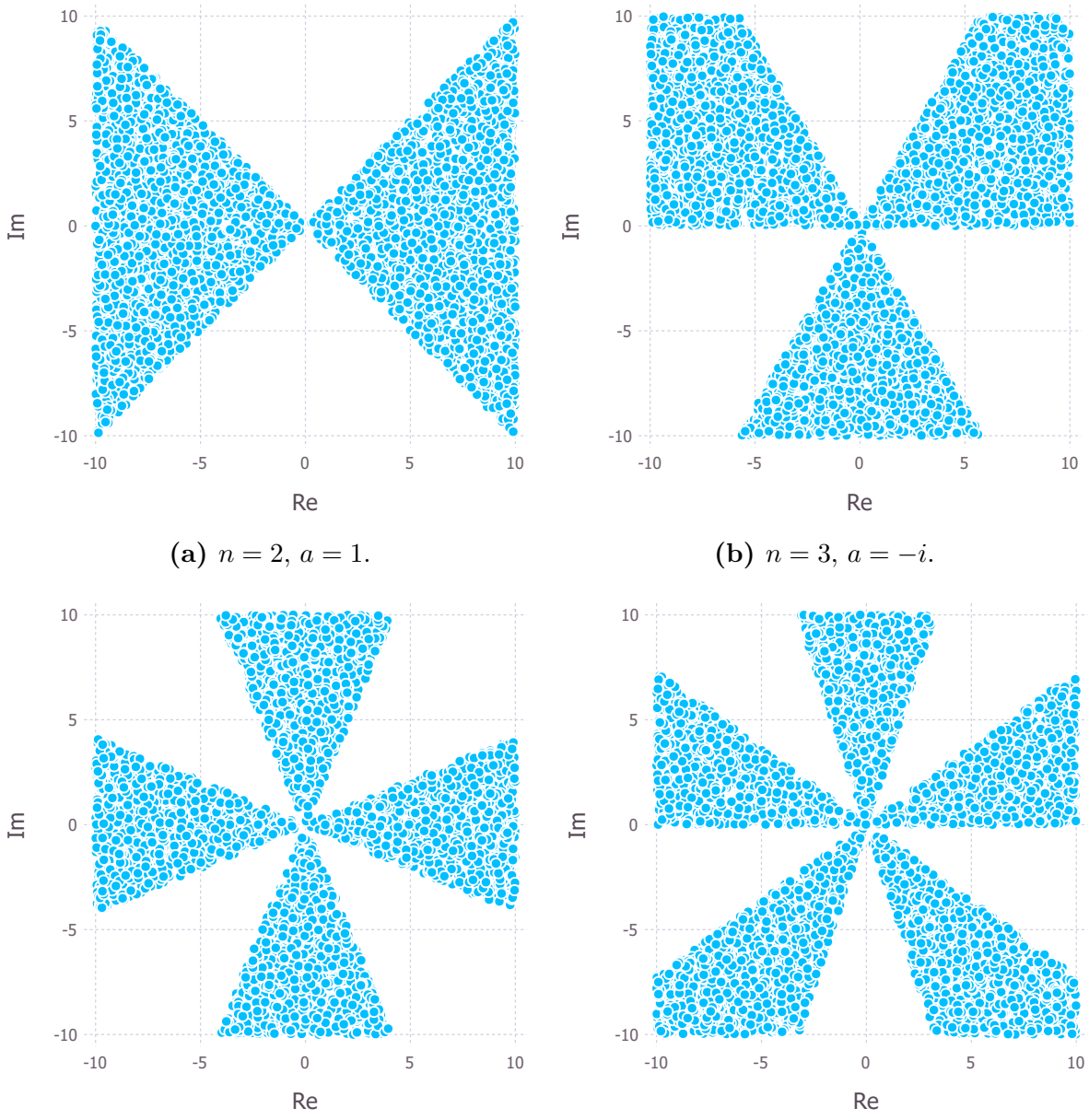
Figure 4 shows some simulations of the region $\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}$. Note that the region consists of a number of connected components, which we henceforth refer to as sectors.

Deforming contour backbone to avoid the integrands' poles

The boundaries of the sectors found above form the "backbones" of the contours Γ_a^+ and Γ_a^-. We proceed to turn these "backbones" into Γ_a^+, Γ_a^- by deforming them to avoid the poles of the integrands F_λ^+ and F_λ^-, which are the zeros of $\Delta(\lambda)$.

Before going into the technicalities of the contour deformation, we first draw attention to a modification of the mathematical construction of Γ in the actual implementation of the algorithm. In (3.6), Γ is defined on the entire complex plane; that is, we can have λ with arbitrarily large modulus. In the actual implementation, however, we choose a sufficiently large real number d to represent the modulus of complex infinity in the algorithm's context. That is, we restrict the mathematical construction to the disk $D(0, d)$. As the choice of d potentially implies a tradeoff between computational cost and numerical accuracy, it should be chosen with regard to the error tolerance of the computational task at hand. The figures in this report and the documentation of the implementation of the Fokas method [16] are obtained with $d = 10$ for clearer illustration. Note that the original infinite contour integrals are understood as improper integrals which, whenever they exist, are equal to their principal values, namely the limits of the respective integrals as the integration bounds tend to infinity. Truncating within $D(0, d)$ and expecting convergence as $d \to \infty$ is therefore legitimate.

By the theory of exponential polynomials [14], $\Delta(\lambda)$ has infinitely many zeros, yet any finite region contains only finitely many of these zeros. Since we restrict the construction to the finite region $D(0, d)$, we would only be dealing with finitely many zeros of $\Delta(\lambda)$. This is an important fact: One complication that arises in practice is that each circular contour around a zero of $\Delta(\lambda)$ not only cannot overlap with the circle around another zero



(a) $n = 2$, $a = 1$.

(b) $n = 3$, $a = -i$.

(c) $n = 4$, $a = 1$.

(d) $n = 5$, $a = -i$.

Figure 4: Simulation of the region $\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}$ by randomly sampling 10^4 points λ and keeping those that satisfy $\mathrm{Re}(a\lambda^n) > 0$.

but also cannot overlap with the boundary of any sector. That is, in Figure 3, the blue and black circles not only cannot overlap with each other, but they also cannot overlap with the red or green dashed lines if the zeros of $\Delta(\lambda)$ at their centers do not lie on the boundaries of the red or green sectors. This implies that the 5ϵ introduced in section 3.2 in fact needs to be the minimum of the infimum of the pairwise distances between distinct zeros of $\Delta(\lambda)$ and the infimum of distances between each zero that is exterior to all sectors and the boundary of each sector. The theory of exponential polynomials [14] guarantees that the former infimum is positive, but there is no such guarantee for the latter infimum. However, precisely because we are working with a finite number of zeros of $\Delta(\lambda)$ in $D(0, d)$, the latter infimum is positive, and so is ϵ.

To see that our choice of ϵ is valid, suppose 5ϵ is the minimum of the two infima described above. Then the circle of radius ϵ around a zero of $\Delta(\lambda)$ does not overlap with any sector boundary. Moreover, the contours around any two distinct zeros of $\Delta(\lambda)$ do not overlap. Indeed: In Figure 5, suppose the radius of the blue circle around a zero of $\Delta(\lambda)$ is ϵ and the distance between the blue circle and the red dashed curve around it is again ϵ. Then since the distance between any two distinct zeros of $\Delta(\lambda)$ is no less than 5ϵ, the blue circle together with the red dashed curve around it is still of distance $5\epsilon - 2\epsilon \cdot 2 = \epsilon$ from the red dashed curve and the blue circle surrounding the nearest zero of $\Delta(\lambda)$. Thus, our choice of ϵ ensures that no contour around a zero of $\Delta(\lambda)$ is "overwritten" by the contour around another zero.

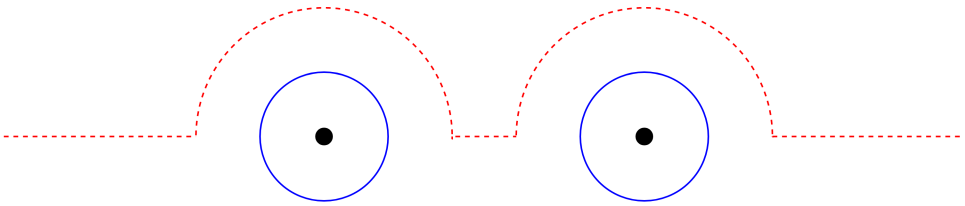


Figure 5: Two distinct zeros of $\Delta(\lambda)$ that are 5ϵ apart. The blue circles and red dashed contours are as in Figure 3. The radius of the blue circles, the distance between each blue circle and the red dashed curve around it, and the distance between the two red dashed curves, are all ϵ.

Suppose for now that we have been given finitely many zeros of $\Delta(\lambda)$ in $D(0, d)$ (we will show how to approximate these zeros at the end of this section).

In the complex plane, a ray (straight half-line) emanating from the origin is characterized by the argument of any point on the ray. From Figure 4, we note that each sector in the region $\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}$ is characterized by the arguments of the two rays that mark its boundaries, namely the starting ray and the ending ray, such that the if the sector is traversed counterclockwise from one end to the other, the starting ray will be traversed before the ending ray. For example, with $n = 3$ and $a = -i$, as shown in section 3.2.2, the region $\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}$ is characterized by the rays with arguments $0, \frac{\pi}{3}, \frac{2}{3}\pi, \pi, \frac{4}{3}\pi, \frac{5}{3}\pi$, where $0, \frac{2}{3}\pi, \frac{4}{3}\pi$ are the angles of the starting rays, and $\frac{\pi}{3}, \pi, \frac{5}{3}\pi$ are the angles of the ending rays.

Note that each sector is assigned to Γ_a^+ or Γ_a^- depending on whether it belongs to the upper or the lower half plane. As shown in Figure 8, if a sector overlaps with the real line, we divide it into the upper and lower half planes, which can then be assigned to Γ_a^+ and Γ_a^-, respectively. In the implementation, this is done by modifying the starting and

ending rays that characterize the sector so that it is split into two sub-sectors, one ending at the real line and the other starting at it.

The contours $\Gamma_a^{\pm}$ are built from these rays with possible deformations to avoid zeros of $\Delta(\lambda)$. Here we make another modification of the mathematical construction in (3.6) to save computational cost. We note that the contours $\Gamma_a^{\pm}$ and $\Gamma_0^{\pm}$ defined in (3.6) lead to partial cancellation, and deformation is in fact only necessary if a zero lies on the boundary of some sector. Indeed: As illustrated in Figure 3, the red and blue dashed lines do not need to be deformed to avoid zeros exterior to all sectors because they are already outside the sectors. Moreover, zeros interior to any sector can be ignored, since integrating over the blue circle around the zero counterclockwise cancels with integrating over the interior red dashed circle around the zero clockwise. For a zero that lies on the boundary of the sector, half of the blue circle around it that is interior to the sector cancels out with the red dashed curve around it, but the other half that is exterior to the sector does not cancel with anything. In this case, we deform the ray on which the zero lies to include the half of the blue circle that does not cancel.

On a side note, the way we deform the contours described above implies that we can choose ϵ to be $\frac{1}{4}$ the minimum of the pairwise distances between distinct zeros of $\Delta(\lambda)$ and the distances between any zero to any sector boundary, instead of $\frac{1}{5}$ as before. Indeed: Since we are merging the blue circle into the red dashed curve, the scenario in Figure 5 would not occur. Instead, the scenario that puts the most constraint on ϵ occurs when a zero is at the origin, and as shown in Figure 6, this scenario only requires that the two distinct zeros are 4ϵ apart. Since zeros of $\Delta(\lambda)$ are poles of F_λ^+, F_λ^- in (3.5), the values of F_λ^+, F_λ^- may easily blow up near the zeros, thereby creating numerical instability. Thus, we use the new choice of ϵ in the actual implementation to make the contours stay further away from the zeros. Figure 7 shows the contour Γ for some examples, and Figure 8 shows each component of Γ of Figure 7(a) separately.

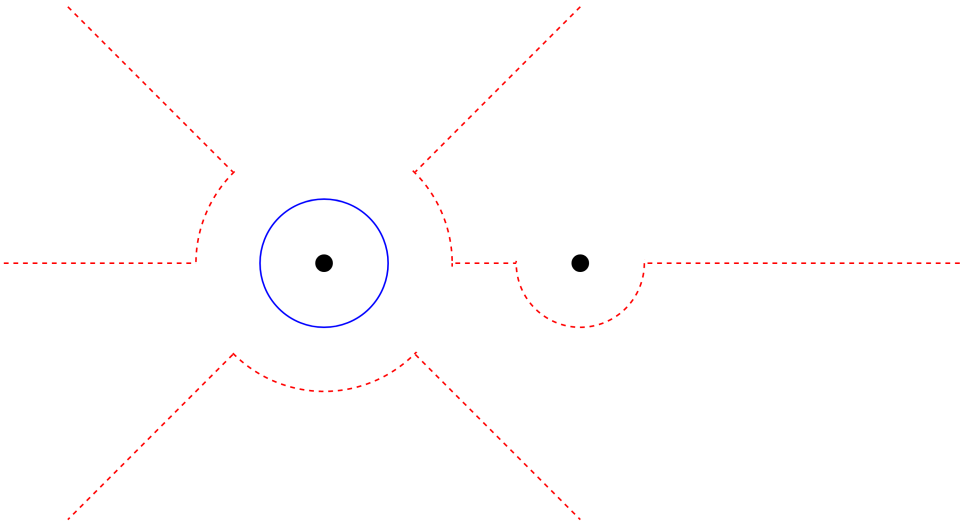
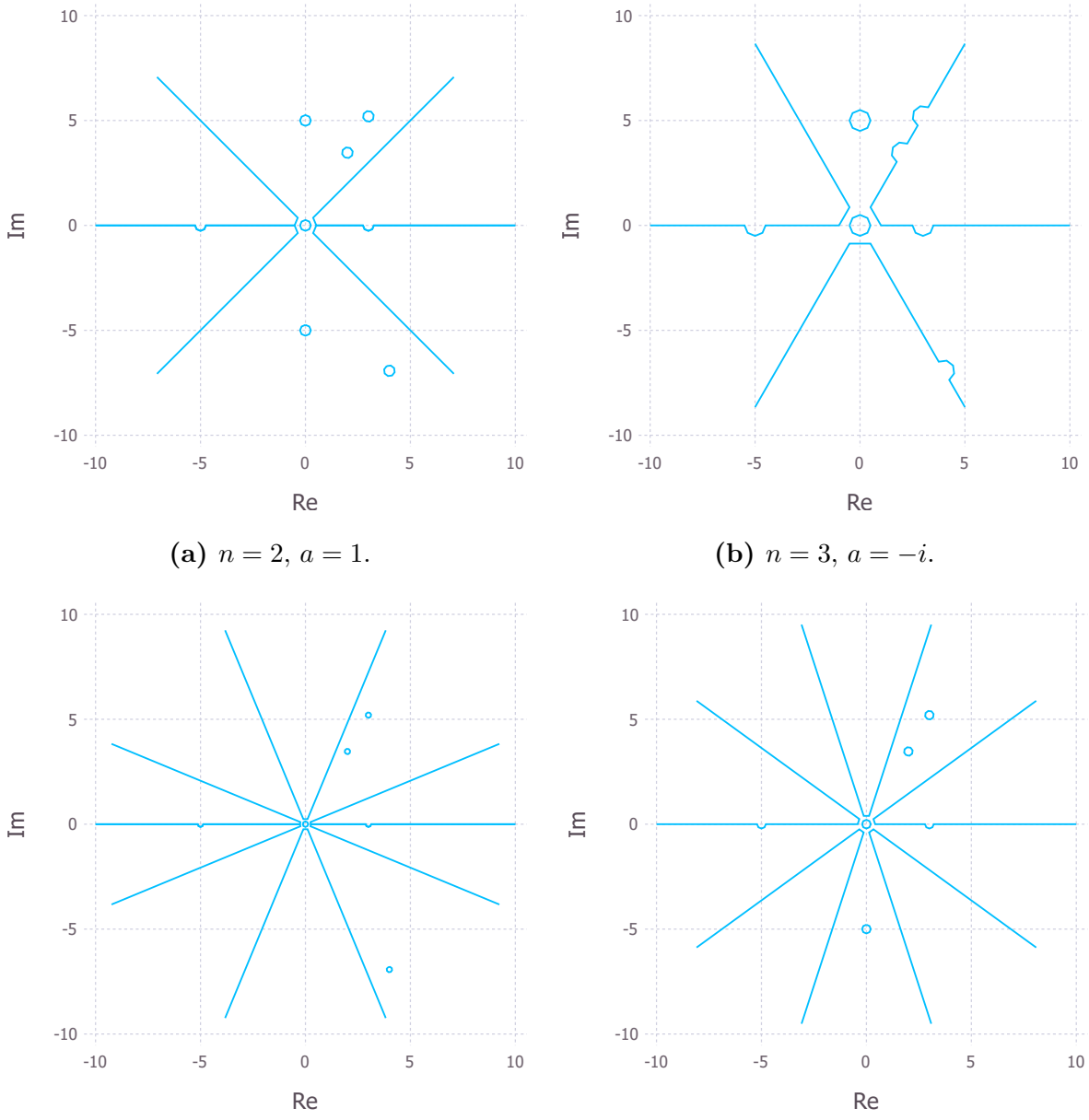


Figure 6: Two distinct zeros of $\Delta(\lambda)$ that are 4ϵ apart. The zero on the left is at the origin. The blue circles and red dashed contours are as in Figure 3 (though not drawn to scale here). The radius of the blue circles, the distance between the blue circle and the red dashed curve around it, and the distance between the two red dashed curves, are all ϵ.

The construction of Γ_a^+, Γ_a^-, Γ_0^+, and Γ_0^- is described as follows. In the implementation, each contour in Γ is encoded by an array of points listed in the order of integration. By Figure 3, we integrate over each contour in $\Gamma_a^{\pm}$ from the ending ray to the starting ray, and



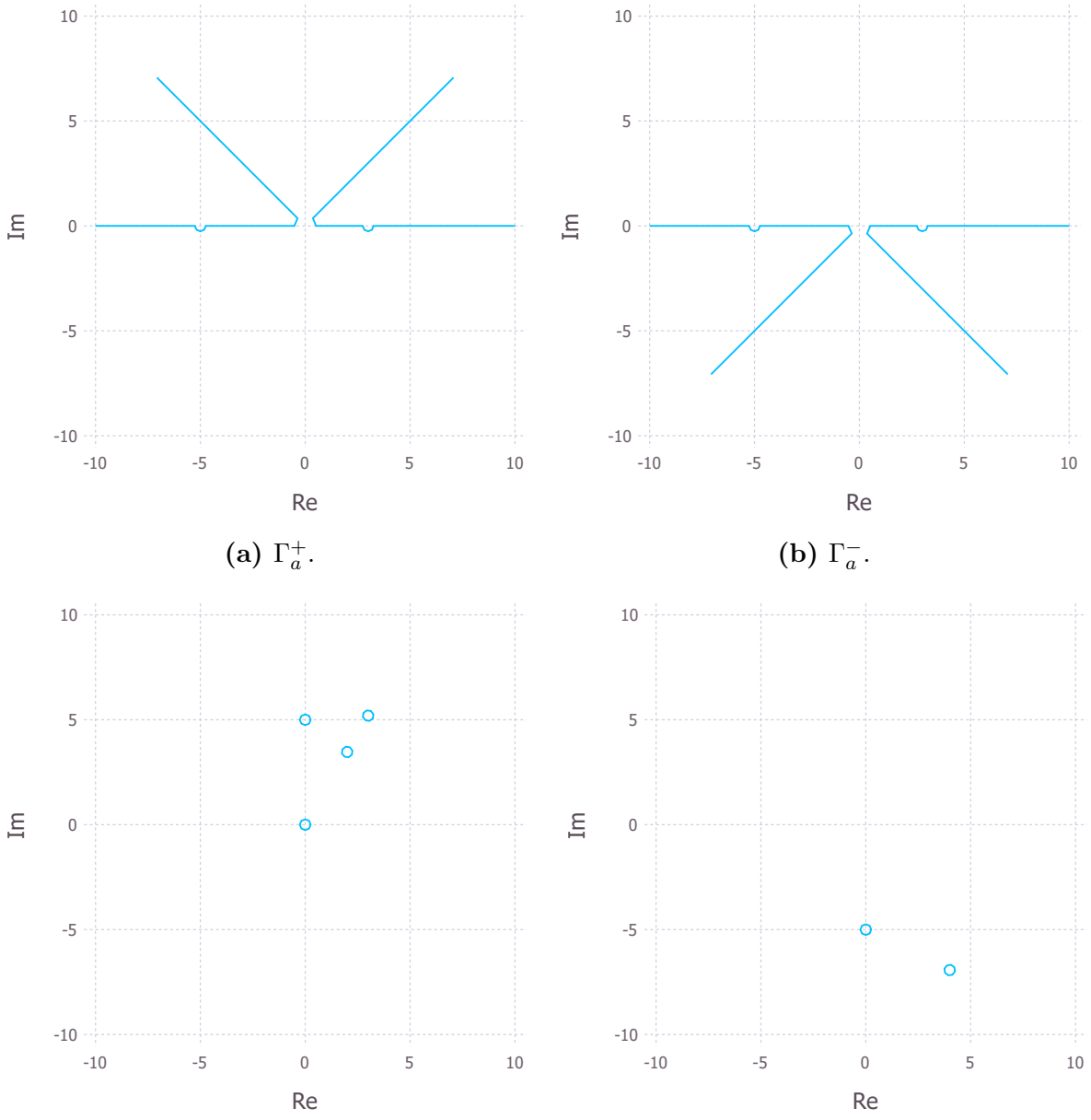
(a) $n = 2$, $a = 1$.

(b) $n = 3$, $a = -i$.

(c) $n = 4$, $a = 1$.

(d) $n = 5$, $a = -i$.

Figure 7: Γ with with zeros of $\Delta(\lambda)$ at $3 + 3\sqrt{3}i$, $2 + 2\sqrt{3}i$, $0 + 0i$, $0 + 5i$, $0 - 5i$, 3, -5, and $4 - 4\sqrt{3}i$. Note that Γ_a^+ are deformed to avoid zeros on the sectors' boundaries.



(a) Γ_a^+. **(b)** Γ_a^-.

(c) Γ_0^+. **(d)** Γ_0^-.

Figure 8: Components of Γ with $n = 2$, $a = 1$, and the same zeros of $\Delta(\lambda)$ as in Figure 7. Note that the sectors are split at the real line into the upper and lower half planes.

each contour in $\Gamma_0^{\pm}$ counterclockwise. Thus, in constructing the contours, for each sector, we initialize its boundary contour by an array of three points, namely the point on the ending ray with distance d from the origin, the origin itself, and the point on the starting ray with modulus d. We add these initial sector boundary contours to $\Gamma_a^{\pm}$ depending on whether the sectors are in the upper or lower half planes. Then, for each zero of $\Delta(\lambda)$ that is not at the origin, if it is on the boundary of some sector, we deform the boundary contour of that sector to include a "bulge" that is the exterior half of an N-gon of radius ϵ around the zero, with the vertices listed counterclockwise. If the zero is exterior to all sectors, we add an N-gon contour around it to $\Gamma_0^{\pm}$, depending on whether the zero is in the upper or lower half plane. If the zero is interior to any sector, we ignore it, since its contribution to the contour integral will be cancelled out, as explained before. Finally, if there is a zero at the origin, we draw an N-gon around it and deform the boundary contours of all sectors to avoid the N-gon.

Approximating the poles of the integrands
As promised, we now describe a method to approximate the poles of F_λ^+ and F_λ^-, i.e., the zeros of $\Delta(\lambda)$, in the finite region $D(0,d)$.

Writing $\Delta(\lambda) = \mathrm{Re}(\Delta)(\lambda) + i\mathrm{Im}(\Delta)(\lambda)$ for $\mathrm{Re}(\Delta), \mathrm{Im}(\Delta) : \mathbb{C} \to \mathbb{R}$, we note that λ_0 is a root of $\Delta(\lambda)$ if and only if it is both a root of $\mathrm{Re}(\Delta)(\lambda)$ and a root of $\mathrm{Im}(\Delta)(\lambda)$. Thus, to find zeros of $\Delta(\lambda)$, we aim to solve simultaneously

$$\mathrm{Re}(\Delta)(\lambda) = 0, \tag{3.9a}$$
$$\mathrm{Im}(\Delta)(\lambda) = 0. \tag{3.9b}$$

We approximate the solutions to (3.9) by visualizing their corresponding level curves. In the examples shown in Figure 9, the red lines correspond to the zeros of $\mathrm{Re}(\Delta)(\lambda)$, and the blue lines correspond to those of $\mathrm{Im}(\Delta)(\lambda)$. We can approximately locate the zeros of $\Delta(\lambda)$ at the intersections of the red and blue lines.

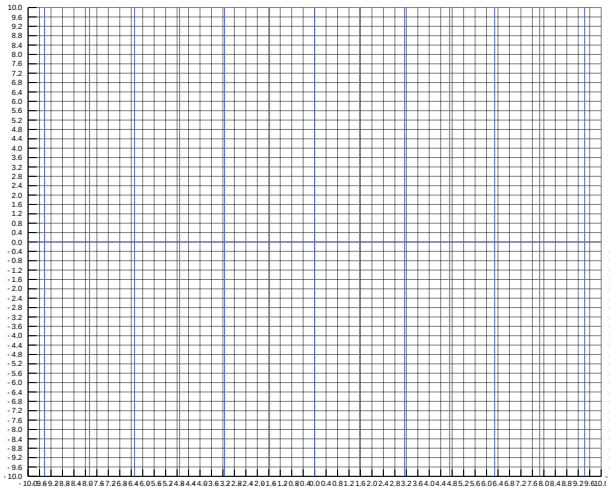
The above method still requires a human to read the level curve plots and record the zeros of $\Delta(\lambda)$ in an array, so that it can be used as an input to the algorithm that produces Γ. Yet this does not introduce much inaccuracy: Recall that when constructing Γ, we need to deform the contours to avoid zeros of $\Delta(\lambda)$ with N-gons of radius ϵ. Thus, there is relatively high tolerance for our approximation of the locations of the zeros.

4 Implementation

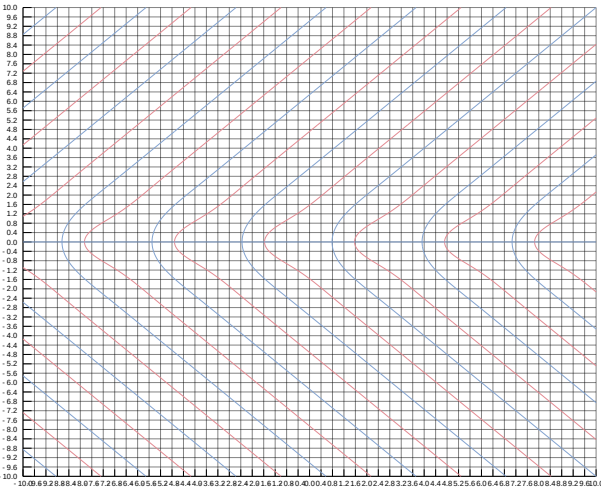
4.1 Overview

The above algorithm is implemented in Julia 0.6.4. Packages used are "SymPy" [17], "sympy" [18], "Distributions" [19], "ApproxFun" [20], "Roots" [21], "QuadGK" [22], "Plots" [23], "Gadfly" [24], and "PyPlot" [25]. Documentation with examples can be found at [16], with possible minor differences in notation from section 3.2.

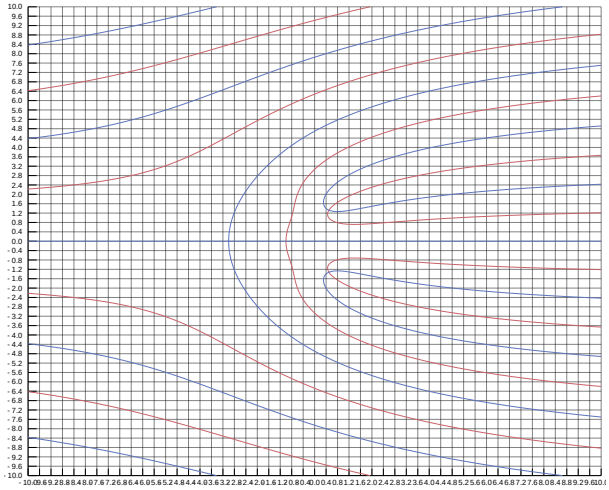
As mentioned near the end of section 1.1, the implementation aims at providing computer aid alongside human judgment in the process of using the Fokas method to solve IBVPs.



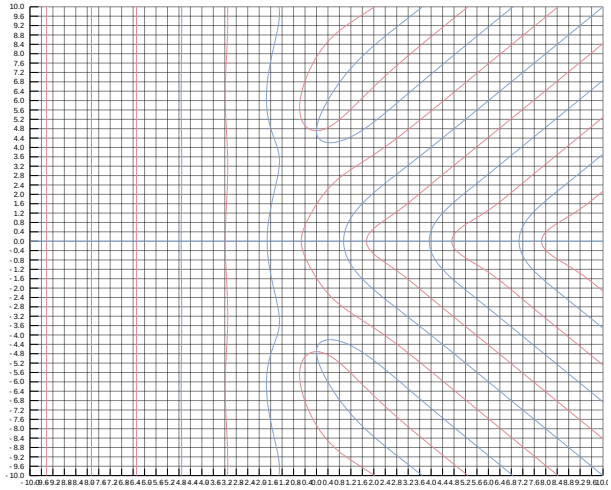
(a) $\Delta(\lambda) = \cos(\lambda)$.



(b) $\Delta(\lambda) = \cos(\lambda)e^{\lambda}$.



(c) $\Delta(\lambda) = (\lambda^3 + \lambda + 2)e^{\lambda}$.



(d) $\Delta(\lambda) = \cos(\lambda)e^{\lambda} + \sin\lambda$.

Figure 9: Level curves corresponding to (3.9).

4.2 Sample usage

We illustrate the utilities of the implementation using two cases of sample usage below. More details can be found in the documentation [16].

4.2.1 Solving IBVP

In this section, we show how the implementation provides computer aid in the process of applying the Fokas method.

Consider the heat equation IBVP

$$q_t - q_{xx} = 0 \qquad \forall (x,t) \in (0,1) \times (0,T) \tag{4.1a}$$
$$q(x,0) = f(x) \qquad \forall x \in [0,1] \tag{4.1b}$$
$$q(0,t) - q(1,t) = 0 \qquad \forall t \in [0,T] \tag{4.1c}$$
$$q_x(0,t) - q_x(1,t) = 0 \qquad \forall t \in [0,T], \tag{4.1d}$$

where $f(x)$ also satisfies equations (4.1c)–(4.1d).

Rewriting the IBVP in the form (1.7), we have $n = 2$, $a = 1$,

$$S = (-i)^2 \frac{d^2}{dx^2} = -\frac{d^2}{dx^2},$$

$$B_1\phi = 1 \cdot \varphi(0) + (-1) \cdot \varphi(1) + 0 \cdot \varphi^{(1)}(0) + 0 \cdot \varphi^{(1)}(1)$$
$$B_2\phi = 0 \cdot \varphi(0) + 0 \cdot \varphi(1) + 1 \cdot \varphi^{(1)}(0) + (-1) \cdot \varphi^{(1)}(1),$$

and

$$\Phi = \{\phi \in C^\infty[0,1] : \, B_j\phi = 0 \, \forall j \in \{1,2\}\}.$$

Using the notation in section 3.1, the two matrices associated with the vector boundary form corresponding to the above boundary conditions are

$$M = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad N = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}.$$

We choose $f(x) = \sin(2\pi x)$ to be the initial datum. Then $f(x)$ satisfies

$$Uf = \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} f(0) \\ f'(0) \\ f(1) \\ f'(1) \end{bmatrix} = 0.$$

By (2.14), $f \in \Phi$, as required.

The adjoint vector boundary form found by the algorithm outlined in section 3.1 is characterized by the matrices

$$b^\star = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \tag{4.2a}$$
$$\beta^\star = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \tag{4.2b}$$

From (4.2), we compute $\Delta(\lambda)$ in (3.4) to be

$$\Delta(\lambda) = 8i\lambda \sin^2\left(\frac{\lambda}{2}\right), \tag{4.3}$$

and $F_\lambda^+(f)$, $F_\lambda^-(f)$ in (3.5) to be

$$F_\lambda^+(f) = \frac{\hat{f}(\lambda)e^{i\lambda}}{2\pi(e^{i\lambda}-1)} \tag{4.4a}$$

$$F_\lambda^-(f) = \frac{\hat{f}(\lambda)}{2\pi(e^{i\lambda}-1)}, \tag{4.4b}$$

where $\hat{f}(\lambda) = \int_0^1 e^{i\lambda x} f(x)\,dx$ is approximated using the method in section 3.2.1.

From the level curves corresponding to (3.9) in Figure 10, we see that the zeros of $\Delta(\lambda)$ are $-2\pi, 0, 2\pi$. With this information, we find the contours Γ to be as in Figure 11.

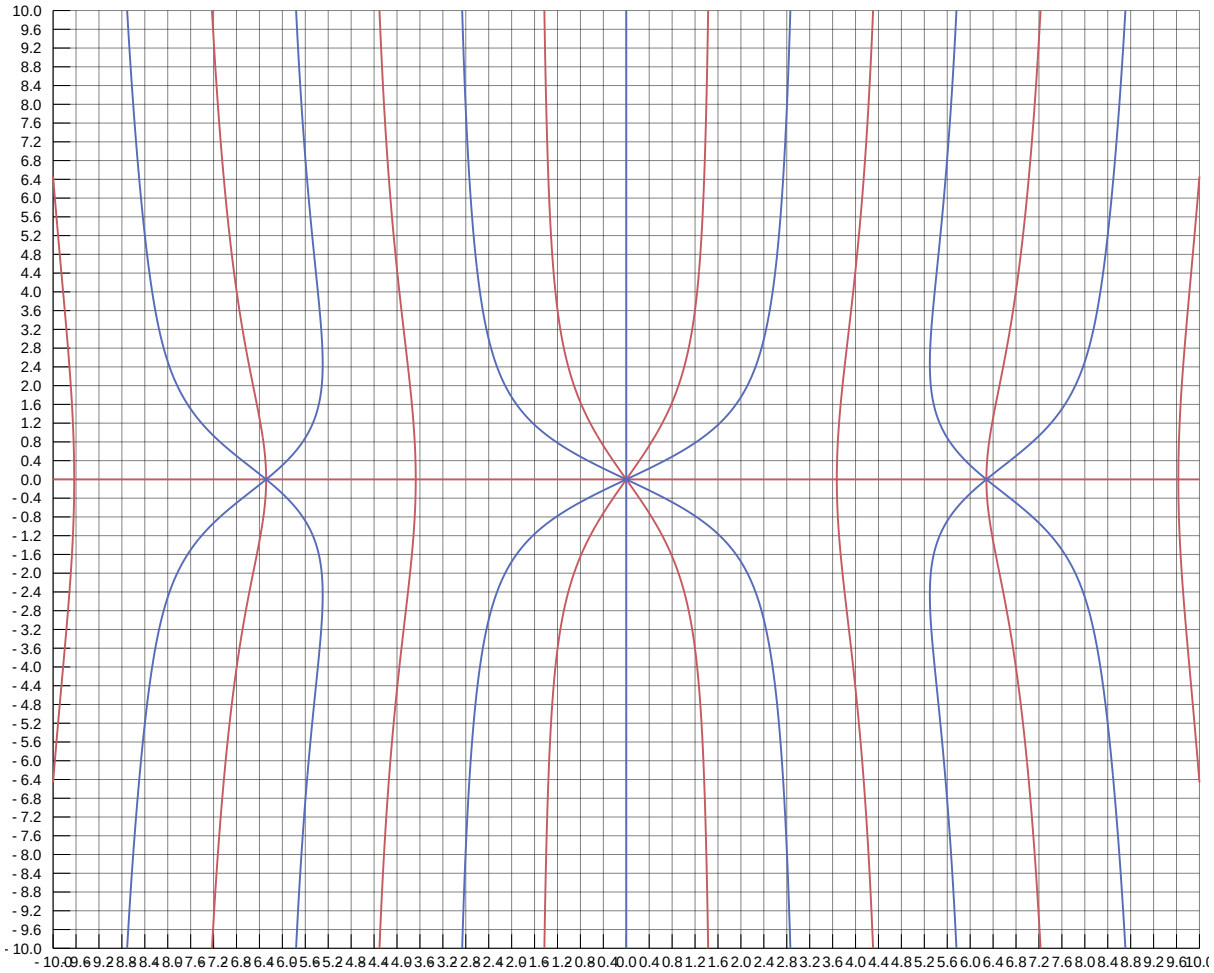


Figure 10: Level curves corresponding to (3.9) with $\Delta(\lambda)$ defined in (4.3).

As shown in equation (3.8), to compute $q(x,t)$, we need to evaluate $e^{i\lambda x}e^{-a\lambda^n t}F_\lambda^\pm(f)$ over the contours $\Gamma_a^\pm$ and $\Gamma_0^\pm$, respectively; call this the outer integral. We note that the inner integral $\int_0^1 e^{i\alpha^{l-1}\lambda x} f(x)\,dx$ in (3.5) depends on both λ and f. One consequence is that if F_λ^+, F_λ^- are to be implemented as functions without symbolic expressions, they

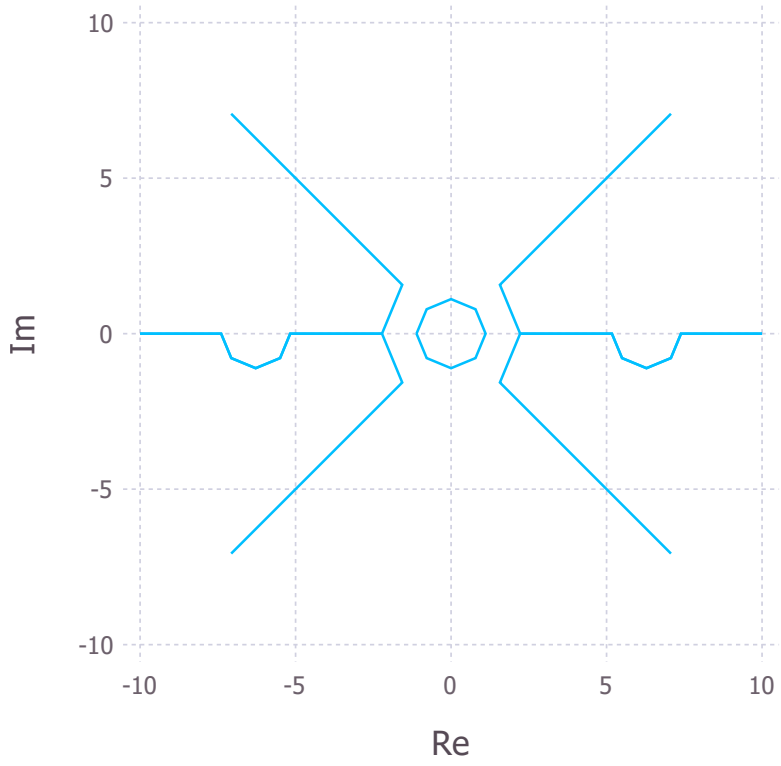


Figure 11: The Γ contour.

each need to take both λ and f as arguments. But doing so results in unnecessary computational cost: The outer integral is over λ only, that is, when evaluating it, λ changes while f does not. But once λ changes, the inner integral also needs to be re-calculated, and because it depends on f and λ, the procedure to approximate the integral described in section 3.2.1 would need to be repeated. As a result, when evaluating $q(x,t)$, the Chebyshev approximation of f is re-calculated at each point in the Γ contour even though f does not change throughout the process. Current implementation of the Fokas method avoids such unnecessary computational cost by obtaining the explicit symbolic formulas of F_λ^+, F_λ^- that depend on λ only, namely (4.4), with $\hat{f}(\lambda)$ replaced by the approximation of $\int_0^1 e^{i\lambda x} f(x)\,dx$ obtained in section 3.2.1 as symbolic expressions in λ. In this way, the components of the outer integral that depend on f are evaluated only once.

In practice, we would convert the symbolic formulas into function objects, because in Julia, function objects are evaluated much faster than symbolic objects. More recent versions of Julia have parsers that perform the conversion. In Julia 0.6.4 in which the current implementation is based (for reasons explained in the last paragraph in section 1.1), however, no such parser exists, and conversion needs to be done manually, namely to create the corresponding function objects by typing in the symbolic formulas in the function definition. Having done so, current implementation of the Fokas method allows evaluating $q(x,t)$ at a given $(x_0,t_0) \in (0,1)\times(0,T)$ within 20 seconds with the modulus of complex infinity set as 10, and within 1 minute with the modulus of complex infinity set as 50 (which is a more reasonable value regarding numerical accuracy as explained in section 3.2.2).

As a side note, the solution $q(x,t)$ computed above using equation (3.8) corresponds to the separated solution of the heat equation [8] in the following sense. Using Cauchy's theorem and Jordan's lemma from complex analysis, it can be shown that integration over the Γ contour in Figure 11 reduces to integration over closed contours around the poles of F_λ^+ and F_λ^-, i.e., the zeros of $\Delta(\lambda)$ in Figure 10. That is, $q(x,t)$ reduces to a sum of contour integrals around zeros of $\Delta(\lambda)$, and using the residue theorem, these contour integrals can be shown to correspond to the eigenfunctions of Sturm-Liouville BVP related to the heat equation IBVP. Since $\Delta(\lambda)$ have infinitely many zeros on the real line, as the estimate of the modulus of complex infinity d tends to ∞, Γ would effectively consist of infinitely many closed contours centered on the real line, much like the blue circles on $\mathrm{Re}(\lambda)$ in Figure 3, but extending to ∞ in both directions. As a result, $q(x,t)$ would become an infinite series of contour integrals, which is none other than the separated solution of the heat equation of the form

$$q(x,t) = \sum_{n=1}^{\infty} A_n \phi_n(x) e^{-\lambda_n K t},$$

where A_n are Fourier coefficients of the initial datum $f(x)$, λ_n the eigenvalues of the Sturm-Liouville problem, and $\phi_n(x)$ the corresponding eigenfunctions. Such correspondence to the separated solution makes sense since the Fokas transform effectively separates the spatial and temporal components of the IBVP.

4.2.2 Symbolic features

In this section, we illustrate how the symbolic formulas provided by the implementation can be useful.

Applying the Fokas method to IBVPs and beyond depends on two technical lemmas, one concerning the positions of the poles of F_λ^+, F_λ^- (i.e., zeros of $\Delta(\lambda)$), the other concerning the asymptotic decay of F_λ^+, F_λ^-. These lemmas are first described in [5] for IBVPs, and they may assume variations for different classes of problems such as those described in the beginning of section 5. The lemmas's precise roles are more clearly articulated in [10], which also describes the extension of the Fokas method to a broader class of problems. Thus, in proving these lemmas or their variations, it would be helpful to have the symbolic formulas for F_λ^+, F_λ^-.

For the IBVPs (1.2) and (1.3), the formulas for F_λ^+ and F_λ^- have been computed by hand in [1, p. 1-4]. Symbolic formulas for the same objects have been found by the implementation of the Fokas method following the steps outlined in section 4.2.1, with S, a as described in section 1.2, and

$$M = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad N = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & -2 & 0 \end{bmatrix}$$

in (1.2), and

$$M = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad N = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

in (1.3). The symbolic formulas found by the implementation, though not simplified to forms pleasant to the human eye due to limitations of the Julia packages used, have been

verified to be equivalent to those derived by hand in [1] by comparing the coefficients of $\hat{f}(\alpha^{l-1}\lambda) = \int_0^1 e^{-i\alpha^{l-1}\lambda x} f(x)\,dx$ in (3.5) evaluated at 100 random values of $\lambda \in \mathbb{C}$ avoiding any zeros of $\Delta(\lambda)$.

5 Discussion

5.1 Extension to other problems

This project concerns applying the Fokas method to solving IBVPs. With appropriate adjustments, the Fokas method can be extended to other types of problems, such as multipoint problems [26], nonlocal problems [10], interface problems [27] concerning KdV equations and more [28], and PDEs of fractional orders [29]. Correspondingly, the implementation of the Fokas method in this project may be extended to problems beyond IBVPs: While necessary adjustments need to be made, usefulness of the implementation's functionalities such as those described in section 4.2.2 should remain generalizable to applications of the Fokas method to other settings.

5.2 Possible improvements

Currently, this project's implementation of the Fokas method [16] supplies utilities such as contour visualization, symbolic formulas derivation, and numerical evaluation that significantly reduce the time and effort in applying the Fokas method compared to working by hand. Possible directions for further improvement involve wider coverage of automated functionalities and faster computation speed.

5.2.1 Automatically approximating poles of the integrands

As mentioned in section 3.2.2, to approximate the poles of F_λ^+ and F_λ^-, i.e., zeros of $\Delta(\lambda)$, in the region $D(0,d)$ (where d is the number representing the modulus of complex infinity), human judgement is still needed to visually locate the zeros as the intersections of the level curves of $\mathrm{Re}(\Delta)(\lambda) = 0$ and $\mathrm{Im}(\Delta)(\lambda) = 0$. This procedure may be automated based on [30], which describes a numerical method to find zeros of an analytic function in a given region using Cauchy's argument principle.

By Cauchy's argument principle, if C is a closed curve, R is the interior of C, and $f(z)$ is analytic in and on C, then the number of zeros of $f(z)$ in R is given by

$$N_z := \frac{1}{2\pi i}\int_C \frac{f'(z)}{f(z)}\,dz.$$

As mentioned in section 3.2, $\Delta(\lambda)$ is an exponential polynomial, and so it is analytic. By the above result, the number of zeros of $\Delta(\lambda)$ in $D(0,d)$ is given by

$$\frac{1}{2\pi i}\int_{C(0,d)} \frac{\Delta'(\lambda)}{\Delta(\lambda)}\,d\lambda.$$

Thus, to approximate the zeros of $\Delta(\lambda)$, we may divide the region $D(0,d)$ into sub-regions, find the number of zeros in each region, discard those sub-regions that do not contain any zeros, and proceed iteratively, until we obtain N_z sub-regions whose radii are within a certain pre-determined tolerance level, each trapping exactly one zero of

$\Delta(\lambda)$. Alternatively, one may strictly follow the method in [30], which starts by dividing the region into sub-regions until each sub-region contains no more than a pre-determined number n_z of zeros. Then, zeros in any given sub-region (if any) are found by first constructing an n_z-degree polynomial with the same zeros as $\Delta(\lambda)$ in that sub-region, and then finding the zeros of this constructed polynomial by exploiting the rich collection of root-finding algorithms for polynomials.

5.2.2 Computation speed

Although evaluation of the solution $q(x,t)$ at a single point can now be done in less than a minute with a reasonable estimate of the modulus of complex infinity (see the end of section 4.2.1), analyzing the solution in depth usually involves visualizing it, which poses a much higher demand on the evaluation speed of the solution. To plot in reasonable time, evaluation at a single point should ideally be a fraction of a second. The implementation as it is now evaluates $q(x,t)$ as follows. Given $(x_0,t_0) \in (0,1) \times (0,T)$, the integrand $e^{i\lambda x_0}e^{-\alpha\lambda^n t_0}F_\lambda^\pm(f)$ in equation (3.8) is defined as a function of λ, which is then integrated over the four contours Γ_a^+, Γ_a^-, Γ_0^+, and Γ_0^- as in equation (3.8). This means that when attempting to plot $q(x,t)$ over a domain D, at each point $(x_0,t_0) \in D$, a new function corresponding to the integrand is defined, compiled, and evaluated. The problem here is that compilation time could be several orders of magnitude higher than evaluation time, and the more so for complicated functions. For instance, the compilation time issue would be prominent if the Chebyshev approximation of $f(x)$ used in section 3.2.1 has many coefficients; in this case the symbolic formulas for F_λ^+, F_λ^- would be complicated, meaning that they would take much time to compile, making it impractical to plot $q(x,t)$ in reasonable time.

Another problem that contributes to the speed issue is that, if the circular contours around zeros of $\Delta(\lambda)$ have very small diameter ϵ (given our choice of ϵ in section 3.2.2, this would be the case if two distinct zeros are very close to each other, or there is a zero that is close to the boundary of some sector), the integration contours would be very close to the zeros which they are supposed to avoid. As discussed in section 3.2.2, zeros of $\Delta(\lambda)$ are poles of the integrand, so the integrand easily becomes numerically unstable near them, yielding very large numeric values when evaluated. As a result, the integration itself becomes slow.

One possible solution to the above speed issues is to develop a custom integrator tailored to these contour integrals by exploiting the mathematical properties of the integrand and the contour. Analysis of the behaviour of F_λ^+ and F_λ^- over Γ could help identify the components of the integrand that contributes significantly to the integral at different parts of the contour Γ. In this way, we could reduce the time it takes to evaluate $q(x,t)$ by discarding components of the integrand whose contribution to the integral is insignificant.

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