Derivations and Applications for `SimpleDifferentialOperators.jl`

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1 Overview

This package is intended to be a stop-gap while more complete and higher-performance solutions are implemented (in particular, the evolution of `https://github.com/JuliaDiffEq/DiffEqOperators.jl/`). In the meantime, the package hopefully provides a solution for discretizing operators and solving ODEs/PDEs.

The focus is on discretizing linear (and, with some careful checks, affine) operators. In the case of models where the process is non-linear, it is most appropriate for algorithms that iteratively solve linear ODEs/PDEs.

Some notation used throughout the document

- Let $x \in R$ be a variable, and (in general) use a tilde to denote functions or operators on $\mathbb{R}$ whereas we will drop the tilde when discretizing (e.g. $\tilde{f}(\cdot)$ is a continuous function on x while f is a vector of the $\tilde{f}(\cdot)$ function applied to a grid.
- Derivatives are denoted by the operator ∂ and univariate derivatives such as $\partial_x \tilde{v}(x) \equiv \tilde{v}'(x)$.
- Use the vertical bar to denote evaluation at a particular point. That is if $\tilde{B} \equiv \partial_x|_{x=x_0}$ then $\tilde{B}\tilde{v}(x) = \partial_x \tilde{v}(x_0)$, and if $\tilde{B} \equiv 1|_{x=x_0}$ then $\tilde{B}\tilde{v}(x) = \tilde{v}(x_0)$. For the notation, the 1 is simply the identity operator on the function instead of applying a derivative
- Let W_t be the Wiener process with the integral defined by the Ito interpretation

1.1 Linear Differential Equations

ODEs (e.g. Steady State) To understand the class of models that this can support, first look at the sort of ODE that comes out of solving a stationary model. The general pattern is a linear differential operator $\tilde{L}$, a boundary condition operator $\tilde{B}$, the function of interest $\tilde{v}(x)$, and the affine terms $\tilde{f}(\cdot)$ and b. The general problem to solve is to find the $\tilde{v}(x)$ such that.

$$0 = \tilde{L}\tilde{v}(x) - \tilde{f}(x) \tag{1}$$

$$0 = \tilde{B}\tilde{v}(x) - b \tag{2}$$

Motivating Example As a simple example, let

- $x \in [x_{\min}, x_{\max}]$ be a state variable on a domain following the SDE

  $$dx_t = \mu dt + \sigma dW_t$$

  where the variable x_t is reflected at $x_{\min}$ and $x_{\max}$

- The payoffs for state x are a function $\tilde{f}(x)$ defines on the domain
- $\tilde{v}(x)$ as the value of the the stream of payoffs discounted at rate $r > 0$

Then, through standard arguments, the stationary Bellman equation along with boundary conditions is

$$r\tilde{v}(x) = \tilde{f}(x) + \mu\partial_x\tilde{v}(x) + \frac{\sigma^2}{2}\partial_{xx}\tilde{v}(x) \tag{3}$$
$$\partial_x\tilde{v}(x_{\min}) = 0 \tag{4}$$
$$\partial_x\tilde{v}(x_{\max}) = 0 \tag{5}$$

Mapping to the notation of (1) and (2)

$$\tilde{L} \equiv r - \mu\partial_x - \frac{\sigma^2}{2}\partial_{xx} \tag{6}$$
$$\tilde{B} \equiv \begin{bmatrix} \partial_x|_{x=x_{\min}} \\ \partial_x|_{x=x_{\max}} \end{bmatrix} \tag{7}$$
$$b \equiv \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{8}$$

This package will allow you to define the $\tilde{L}$, $\tilde{B}$, and b to solve for a discretization of the $\tilde{v}(x)$ function.

Boundary Conditions The package supports some key boundary conditions used for stochastic processes and ODE/PDEs.

As will become clear in the discretization, whether the boundary condition is homogenous or not (i.e. $= 0$ or $= b > 0$) is important for the numerical methods. To detail a few of the one-dimensional versions of the supported boundary conditions

- Reflecting Barriers (i.e. a homogeneous Neumann Boundary Conditions)

$$\partial_x\tilde{v}(x_{\min}) = 0 \tag{9}$$
$$\partial_x\tilde{v}(x_{\max}) = 0 \tag{10}$$

  or in operator form

$$\tilde{B} \equiv \begin{bmatrix} \partial_x|_{x=x_{\min}} \\ \partial_x|_{x=x_{\max}} \end{bmatrix} \tag{11}$$
$$b \equiv \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{12}$$

- Mixed boundary conditions (i.e a homogeneous Robin Boundary Conditions):

$$\underline{\xi}\tilde{v}(x_{\min}) + \partial_x\tilde{v}(x_{\min}) = 0 \tag{13}$$
$$\overline{\xi}\tilde{v}(x_{\max}) + \partial_x\tilde{v}(x_{\max}) = 0 \tag{14}$$

  Note that when $\underline{\xi} = \overline{\xi} = 0$, this nests the reflecting barriers. In operator form,

$$\tilde{B} \equiv \begin{bmatrix} \partial_x|_{x=x_{\min}} + \underline{\xi}\, 1|_{x=x_{\min}} \\ \partial_x|_{x=x_{\max}} + \overline{\xi}\, 1|_{x=x_{\max}} \end{bmatrix} \tag{15}$$
$$b \equiv \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{16}$$

- Absorbing Barriers (i.e. a homogenous or inhomogeneous Dirichlet Boundary Conditions)

$$\tilde{v}(x_{\min}) = b_1 \tag{17}$$
$$\tilde{v}(x_{\max}) = b_2 \tag{18}$$

In the case of $b_1 = b_2 = 0$, this is homogeneous. In operator form,

$$\tilde{B} \equiv \begin{bmatrix} 1|_{x=x_{\min}} \\ 1|_{x=x_{\max}} \end{bmatrix} \tag{19}$$
$$b \equiv \begin{bmatrix} b_0 \\ b_2 \end{bmatrix} \tag{20}$$

Of course, many models would have different boundary conditions on different sides of the domain, which entails mixing and matching rows in the B and b matrices.

PDEs (i.e. Time-Varying) The motivating example above has no time-variation in any of the parameters, payoffs, or boundary conditions. Consider that the operators, payoffs, and boundary conditions could change over time – which we denote with a t subscript. As a variation on (1) and (2)

$$\partial_t \tilde{v}(t,x) = \tilde{L}(t)\tilde{v}(t,x) - \tilde{f}(t,x) \tag{21}$$
$$0 = \tilde{B}(t)\tilde{v}(t,x) - b(t) \tag{22}$$

Subsect to an initial condition, $\tilde{v}(0,x)$ given or potentially a boundary value, $\tilde{v}(T,x)$ for some T.

This is a linear PDE where the operators, boundary conditions, and payoffs all may change over time.

TODO go back to the motivating example.

2 Discretization

2.1 Notation

This section defines the grids and other notation for the discretization.

- Define an irregular grid $\{x_i\}_{i=0}^{M+1}$ with **boundary nodes**, $x_0 = x_{\min}$ and $x_{M+1} = x_{\max}$. Denote the **extended grid** as $\overline{x} \equiv \{x_i\}_{i=0}^{M+1}$ and the **interior grid**, a collection of nodes excluding the boundary nodes, as $x \equiv \{x_i\}_{i=1}^{M}$.
- Define v as a vector of a function of interest, $\tilde{v}(x)$, evaluated on the interior grid x, i.e., $v = \{\tilde{v}(x_i)\}_{i=1}^{M}$. Likewise, we define a vector of v on the extended grid as $\overline{v} = \{\tilde{v}(\overline{x}_i)\}_{i=0}^{M+1}$.
- Denote the backward and forward distance between the grid points as

$$\Delta_{i,-} \equiv x_i - x_{i-1}, \text{ for } i = 1, \ldots, M+1 \tag{23}$$
$$\Delta_{i,+} \equiv x_{i+1} - x_i, \text{ for } i = 0, \ldots, M \tag{24}$$

- Define the vector of backwards and forwards first differences, padding with $\Delta_{0,-} = \Delta_{M+1,+} = 0$, as

$$\Delta_- \equiv \begin{bmatrix} 0 \\ \mathrm{diff}(z) \end{bmatrix} \in \mathbb{R}^{M+2} \tag{25}$$

$$\Delta_+ \equiv \begin{bmatrix} \mathrm{diff}(z) \\ 0 \end{bmatrix} \in \mathbb{R}^{M+2} \tag{26}$$

Let L_{1-}, L_{1+} be the discretized backward and forward first order differential operators and L_2 be the discretized central difference second order differential operator, all subject to the Neumann boundary conditions in (13) and (14), such that $L_{1-}\bar{v}, L_{1+}\bar{v}$ and $L_2\bar{v}$ represent the first-order (backward and forward) and second-order derivatives of $\tilde{v}(x)$ respectively at x.[1]

3 Discretizing Operators with a Regular Grid

In this section, we study discretization schemes under regular grids, i.e., grids such that $x_{i+1} - x_i = \Delta$ for all $i = 0, ..., M$ for some fixed $\Delta > 0$.

3.1 Extension Operators

Consider constructing first-order derivatives by backward difference ith node:

$$v'_{i,-} = \frac{v_i - v_{i-1}}{\Delta} \tag{27}$$

similarly, using forward differences,

$$v'_{i,+} = \frac{v_{i+1} - v_i}{\Delta} \tag{28}$$

and second-order derivatives,

$$v''_i = \frac{v_{i+1} - 2v_i + v_{i-1}}{\Delta^2} \tag{29}$$

for $i \in \{1, ..., M\}$. Stacking over all first-order derivatives and second order derivatives as vectors,

$$v'_- = \left\{v'_{i,-}\right\}_{i=1}^M \tag{30}$$
$$v'_+ = \left\{v'_{i,+}\right\}_{i=1}^M \tag{31}$$
$$v'' = \left\{v''_i\right\}_{i=1}^M \tag{32}$$

using (27), (28), (29), one can represent the vectors of discretized derivatives as

$$v'_- = L_{1-}\overline{v} \tag{33}$$
$$v'_+ = L_{1+}\overline{v} \tag{34}$$
$$v'' = L_2\overline{v} \tag{35}$$

[1] In the current form, the package composes operators as sparse matrices. Depending on the circumstances, this code will execute slower than a hand-tweaked model creating composed operators directly. In many cases, this wouldn't be a problem, but in some algorithms where operators need to be redefined frequently in tight loops, it might be. In those cases, use the output of this package for test-suites on hand-built discretizations.

with the following **extension operators**:

$$L_{1-} \equiv \frac{1}{\Delta} \begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & \ddots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 & 0 \end{pmatrix}_{M \times (M+2)} \tag{36}$$

$$L_{1+} \equiv \frac{1}{\Delta} \begin{pmatrix} 0 & -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{pmatrix}_{M \times (M+2)} \tag{37}$$

$$L_2 \equiv \frac{1}{\Delta^2} \begin{pmatrix} 1 & -2 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \end{pmatrix}_{M \times (M+2)} \tag{38}$$

which can be defined in more compact forms:

$$L_{1-} \equiv \Delta^{-1} \left[\text{tridiag}(\mathbf{0}_{M-1}, -\mathbf{1}_M, \mathbf{1}_M) \quad \mathbf{0}_M \right] \tag{39}$$

$$L_{1+} \equiv \Delta^{-1} \left[\mathbf{0}_M \quad \text{tridiag}(\mathbf{0}_{M-1}, -\mathbf{1}_M, \mathbf{1}_M) \right] \tag{40}$$

$$L_2 \equiv \frac{1}{\Delta^2} \text{tridiag}^+(\mathbf{1}_M, -2\mathbf{1}_M, \mathbf{1}_M) \tag{41}$$

where $\text{tridiag}(x, y, z)$ is a matrix whose lower, main, upper diagonal vectors are x, y, and z, respectively, and $\text{tridiag}^+(x, y, z)$ is a matrix whose main, upper, and second upper diagonal vectors x, y, and z, respectively.

3.2 Applying Boundary Conditions

Boundary conditions can be applied manually by using operators on extended grids, $\overline{x}$, to find solutions on extended grids. Suppose that we want to solve a system $\tilde{L}\tilde{v}(x) = \tilde{f}(x)$ for $\tilde{v}(x)$ where L is a linear combination of discretized differential operators for some f that represents the values of a function $\tilde{f}(\cdot)$ on discretized interior x. To solve the system under boundary conditions on v, one can construct and solve the following extended system:

$$\begin{bmatrix} L \\ B \end{bmatrix} \overline{v} = \begin{bmatrix} f \\ b \end{bmatrix} \tag{42}$$

with M_E by $(M+2)$ matrix B and M_E-length vector b that represent the current boundary conditions, where M_E is the number of boundary conditions to be applied. The solution of (42), $\tilde{v}(\overline{x})$ can be decomposed into

$$\overline{v} = \begin{bmatrix} \tilde{v}(x_0) \\ v \\ \tilde{v}(x_{M+1}) \end{bmatrix} \tag{43}$$

which also gives the solution for v.

3.2.1 Mixed Boundary Conditions

Recall mixed boundary conditions from (13) and (14). Note that reflecting barrier conditions are special cases with $\overline{\xi} = \underline{\xi} = 0$. Using forward difference and backward difference discretization scheme for the lower bound and upper bound respectively, we have

$$\frac{\overline{v}_1 - \overline{v}_0}{\Delta} - \underline{\xi}\overline{v}_0 = 0 \tag{44}$$

$$\frac{\overline{v}_{M+1} - \overline{v}_M}{\Delta} - \overline{\xi}\overline{v}_{M+1} = 0 \tag{45}$$

Thus, the corresponding boundary condition matrix B is

$$B = \begin{bmatrix} -\frac{1}{\Delta} + \underline{\xi} & \frac{1}{\Delta} & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & -\frac{1}{\Delta} & \frac{1}{\Delta} + \overline{\xi} \end{bmatrix}_{2\times(M+2)} \qquad b = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{46}$$

which provides the identical system as

$$B = \begin{bmatrix} -1 + \underline{\xi}\Delta & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 + \overline{\xi}\Delta \end{bmatrix}_{2\times(M+2)} \qquad b = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{47}$$

Subtracting the first row of $\overline{L}_{1-}$ by the first row of B in (76) multiplied by $(-1 + \underline{\xi}\Delta)^{-1}\Delta^{-1}$ gives, with the corresponding row operation matrix R,

$$RL_{1-} = \frac{1}{\Delta}\begin{pmatrix} 0 & 1 + (-1 + \underline{\xi}\Delta)^{-1} & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & \ddots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 1 & 0 \end{pmatrix}_{M\times(M+2)} \tag{48}$$

note that there is no zero element in the first and last column for nodes on boundaries. Hence, solving the corresponding extended system,

$$\begin{bmatrix} L \\ B \end{bmatrix} = \begin{bmatrix} f \\ b \end{bmatrix} \tag{49}$$

is identical as solving the following system

$$R\begin{bmatrix} L \\ B \end{bmatrix} = R\begin{bmatrix} f \\ b \end{bmatrix} \tag{50}$$

$$= \begin{bmatrix} f \\ b \end{bmatrix} \tag{51}$$

as b is a zero vector so that the row operations R do not change anything on the RHS. Furthermore, limited to the interior, solving v in the system above is identical as solving the following system with an operator L^B on interior nodes:

$$L^B v = f \tag{52}$$

where we have $L = L_{1-}$ and $L^B = L^B_{1-}$ with

$$L^B_{1-} \equiv \frac{1}{\Delta}\begin{pmatrix} 1 + (-1 + \underline{\xi}\Delta)^{-1} & 0 & 0 & \dots & 0 & 0 & 0 \\ -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -1 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{pmatrix}_{M\times M} \tag{53}$$

instead of solving the full system with boundary conditions. Similarly, one can define differential operators on the interior as follows:

$$L_{1-}^B \equiv \frac{1}{\Delta}\begin{pmatrix} 1+(-1+\underline{\xi}\Delta)^{-1} & 0 & 0 & \dots & 0 & 0 & 0 \\ -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -1 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{pmatrix}_{M\times M} \tag{54}$$

$$L_{1+}^B \equiv \frac{1}{\Delta}\begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & -1+(1+\overline{\xi}\Delta)^{-1} \end{pmatrix}_{M\times M} \tag{55}$$

$$L_{2}^B \equiv \frac{1}{\Delta^2}\begin{pmatrix} -2-(-1+\underline{\xi}\Delta)^{-1} & 1 & 0 & \dots & 0 & 0 & 0 \\ 1 & -2 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & -2 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -2+(1+\overline{\xi}\Delta)^{-1} \end{pmatrix}_{M\times M} \tag{56}$$

which can be defined in more compact forms:

$$L_{1-}^B \equiv \text{tridiag}(-\mathbf{1}_{M-1}, \left[1+(-1+\underline{\xi}\Delta)^{-1} \quad \mathbf{1}_{M-1}^T\right]^T, \mathbf{0}_{M-1}) \tag{57}$$

$$L_{1+}^B \equiv \text{tridiag}(\mathbf{0}_{M-1}, \left[-\mathbf{1}_{M-1}^T \quad -1+(1+\overline{\xi}\Delta)^{-1}\right]^T, \mathbf{1}_{M-1}) \tag{58}$$

$$L_{2}^B \equiv \text{tridiag}(\mathbf{1}_{M-1}, \left[-2-(-1+\underline{\xi}\Delta)^{-1} \quad -2\mathbf{1}_{M-2}^T \quad -2+(1+\overline{\xi}\Delta)^{-1}\right]^T, \mathbf{1}_{M-1}) \tag{59}$$

3.2.2 Absorbing Boundary Conditions

To apply an absorbing barrier condition $\tilde{v}(x_{\min}) = S$ for some $S \in \mathbb{R}$, with one reflecting barrier condition on the upper bound $v'(x_{\max}) = 0$, one can use

$$B = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 \end{bmatrix}_{2\times(M+2)} \qquad b = \begin{bmatrix} S \\ 0 \end{bmatrix} \tag{60}$$

Similarly, one can apply an absorbing condition on the upper bound $\tilde{v}(x_{\max}) = S$ for some $S \in \mathbb{R}$ and the

$$B = \begin{bmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 1 \end{bmatrix}_{2\times(M+2)} \qquad b = \begin{bmatrix} 0 \\ S \end{bmatrix} \tag{61}$$

4 Discretizing Operators with a Irregular Grid

4.1 Applying Boundary Conditions

Instead of solving (42) for a value function $\tilde{v}(\overline{x})$ on the extended grid, one can perform Gaussian elimination to reduce the system and solve $\tilde{v}(x)$, which gives the identical solution as the interior of $\tilde{v}(\overline{x})$.

4.2 Irregular grids

Define the vectors of backward and forward distance for interior nodes as follows:

$$\Delta_-^\circ = \{\Delta_{i,-}\}_{i=1}^M \tag{62}$$

$$\Delta_+^\circ = \{\Delta_{i,+}\}_{i=1}^M \tag{63}$$

We can then define the following operators on $\overline{x}$:

$$L_{1-} \equiv \begin{pmatrix} -\Delta_{1,-}^{-1} & \Delta_{1,-}^{-1} & 0 & \dots & 0 & 0 & 0 \\ 0 & -\Delta_{2,-}^{-1} & \Delta_{2,-}^{-1} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \Delta_{M-1,-}^{-1} & 0 & 0 \\ 0 & 0 & 0 & \cdots & -\Delta_{M,-}^{-1} & \Delta_{M,-}^{-1} & 0 \end{pmatrix}_{M\times(M+2)} \tag{64}$$

$$L_{1+} \equiv \begin{pmatrix} 0 & -\Delta_{1,+}^{-1} & \Delta_{1,+}^{-1} & \dots & 0 & 0 & 0 \\ 0 & 0 & -\Delta_{2,+}^{-1} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -\Delta_{M-1,+}^{-1} & \Delta_{M-1,+}^{-1} & 0 \\ 0 & 0 & 0 & \cdots & 0 & -\Delta_{M,+}^{-1} & \Delta_{M,+}^{-1} \end{pmatrix}_{M\times(M+2)} \tag{65}$$

$$L_2 \equiv 2 \begin{pmatrix} (\Delta_{1,+}+\Delta_{1,-})^{-1}\Delta_{1,-}^{-1} & -\Delta_{1,-}^{-1}\Delta_{1,+}^{-1} & (\Delta_{1,+}+\Delta_{1,-})^{-1}\Delta_{i,+}^{-1} & \dots & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & (\Delta_{M,+}+\Delta_{M,-})^{-1}\Delta_{M,-}^{-1} & -\Delta_{M,-}^{-1}\Delta_{M,+}^{-1} & (\Delta_{M,+}+\Delta_{M,-})^{-1}\Delta_{M,+}^{-1} \end{pmatrix}_{M\times(M+2)} \tag{66}$$

Note that we use the following discretization scheme scheme from **?**:

$$v''(x_i) \approx \frac{\Delta_{i,-}\tilde{v}(x_i+\Delta_{i,+}) - (\Delta_{i,+}+\Delta_{i,-})\tilde{v}(x_i) + \Delta_{i,+}\tilde{v}(x_i-\Delta_{i,-})}{\frac{1}{2}(\Delta_{i,+}+\Delta_{i,-})\Delta_{i,+}\Delta_{i,-}}, \text{for } i=1,\dots,M \tag{67}$$

for second-order derivatives.

And one for identity matrix:

$$I \equiv \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{pmatrix}_{M\times(M+2)} \tag{68}$$

Alternatively, in a more compact form, using vectors distances for interior nodes:

$$L_{1-} \equiv \left[\text{tridiag}(\mathbf{0}_{M-1}, -(\Delta_-^\circ)^{-1}, (\Delta_-^\circ)^{-1}) \quad \mathbf{0}_M\right] \tag{69}$$

$$L_{1+} \equiv \left[\mathbf{0}_M \quad \text{tridiag}(\mathbf{0}_{M-1}, -(\Delta_-^\circ)^{-1}, (\Delta_-^\circ)^{-1}) \ \right] \tag{70}$$

$$L_2 \equiv 2 \odot \text{tridiag}^+ \left[(\Delta_-^\circ + \Delta_+^\circ)^{-1} \odot (\Delta_-^\circ)^{-1}, -(\Delta_-^\circ \odot \Delta_+^\circ)^{-1}, (\Delta_-^\circ + \Delta_+^\circ)^{-1} \odot (\Delta_+^\circ)^{-1}\right] \tag{71}$$

$$I \equiv \left[\mathbf{0}_M \quad \text{diag}(\mathbf{1}_M) \quad \mathbf{0}_M\right] \tag{72}$$

4.2.1 Mixed boundary conditions

Recall mixed boundary conditions from (13) and (14). Note that reflecting barrier conditions are special cases with $\overline{\xi} = \underline{\xi} = 0$. Using forward difference and backward difference discretization scheme for the lower bound and upper bound respectively, we have

$$\frac{\overline{v}_1 - \overline{v}_0}{\Delta_{0,+}} - \underline{\xi}\overline{v}_0 = 0 \tag{73}$$

$$\frac{\overline{v}_{M+1} - \overline{v}_M}{\Delta_{M+1,-}} - \overline{\xi}\overline{v}_{M+1} = 0 \tag{74}$$

Thus, the corresponding boundary condition matrix B is

$$B = \begin{bmatrix} -\frac{1}{\Delta_{0,+}} + \underline{\xi} & \frac{1}{\Delta_{0,+}} & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & -\frac{1}{\Delta_{M+1,-}} & \frac{1}{\Delta_{M+1,-}} + \overline{\xi} \end{bmatrix}_{2\times(M+2)} \qquad b = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{75}$$

which provides the identical system as

$$B = \begin{bmatrix} -1 + \underline{\xi}\Delta_{1,-} & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 + \overline{\xi}\Delta_{M,+} \end{bmatrix}_{2\times(M+2)} \qquad b = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{76}$$

since $\Delta_{0,+} = \Delta_{1,-}$ and $\Delta_{M+1,-} = \Delta_{M,+}$

The first columns of all the extension operators above, $\overline{L}_{1-}, \overline{L}_{1+}, \overline{L}_2, \overline{I}$, have non-zero element only in the first rows. Thus, a single Gaussian elimination for the first extension grid will suffice to remove the extended. Likewise, in the last columns of all the extension operators have non-zero element only in the last row.

Subtracting the first row of $\overline{L}_{1-}$ by the first row of B in (76) multiplied by $(-1+\underline{\xi}\Delta_{1,-})^{-1}\Delta_{1,-}^{-1}$ gives, with the corresponding row operation matrix R for Gaussian elimination,

$$RL_{1-} = \begin{pmatrix} 0 & \Delta_{1,-}^{-1}\left[1 + (-1+\underline{\xi}\Delta_{1,-})^{-1}\right] & 0 & \dots & 0 & 0 & 0 \\ 0 & -\Delta_{2,-}^{-1} & \Delta_{2,-}^{-1} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \Delta_{M-1,-}^{-1} & 0 & 0 \\ 0 & 0 & 0 & \dots & -\Delta_{M,-}^{-1} & \Delta_{M,-}^{-1} & 0 \end{pmatrix}_{M\times(M+2)} \tag{77}$$

note that there is no zero element in the first and last column for nodes on boundaries. Hence, solving the corresponding extended system,

$$\begin{bmatrix} L \\ B \end{bmatrix} = \begin{bmatrix} f \\ b \end{bmatrix} \tag{78}$$

is identical as solving the following system

$$R\begin{bmatrix} L \\ B \end{bmatrix} = R\begin{bmatrix} f \\ b \end{bmatrix} \tag{79}$$

$$= \begin{bmatrix} f \\ b \end{bmatrix} \tag{80}$$

as b is a zero vector so that the row operations R do not change anything on the RHS. Furthermore, limited to the interior, solving v in the system above is identical as solving the following system with an operator L^B on interior nodes:

$$L^B v = f \tag{81}$$

where we have $L = L_{1-}$ and $L^B = L^B_{1-}$ with

$$L^B_{1-} \equiv \begin{pmatrix} \Delta^{-1}_{1,-}[1+(-1+\underline{\xi}\Delta_{1,-})]^{-1} & 0 & 0 & \dots & 0 & 0 & 0 \\ -\Delta^{-1}_{2,-} & \Delta^{-1}_{2,-} & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -\Delta^{-1}_{M-1,-} & \Delta^{-1}_{M-1,-} & 0 \\ 0 & 0 & 0 & \cdots & 0 & -\Delta^{-1}_{M,-} & \Delta^{-1}_{M,-} \end{pmatrix}_{M\times M} \tag{82}$$

instead of solving the full system with boundary conditions. Similarly, one can define differential operators on the interior as follows:

$$L^B_{1-} \equiv \begin{pmatrix} \Delta^{-1}_{1,-}[1+(-1+\underline{\xi}\Delta_{1,-})^{-1}] & 0 & 0 & \dots & 0 & 0 & 0 \\ -\Delta^{-1}_{2,-} & \Delta^{-1}_{2,-} & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -\Delta^{-1}_{M-1,-} & \Delta^{-1}_{M-1,-} & 0 \\ 0 & 0 & 0 & \cdots & 0 & -\Delta^{-1}_{M,-} & \Delta^{-1}_{M,-} \end{pmatrix}_{M\times M} \tag{83}$$

$$L^B_{1+} \equiv \begin{pmatrix} -\Delta^{-1}_{1,+} & \Delta^{-1}_{1,+} & 0 & \dots & 0 & 0 & 0 \\ 0 & -\Delta^{-1}_{2,+} & \Delta^{-1}_{2,+} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & -\Delta^{-1}_{M-1,+} & \Delta^{-1}_{M-1,+} \\ 0 & 0 & 0 & \dots & 0 & 0 & \Delta^{-1}_{M,+}[-1+(1+\overline{\xi}\Delta_{M,+})^{-1}] \end{pmatrix}_{M\times M} \tag{84}$$

$$L^B_2 \equiv 2\begin{pmatrix} \Xi_1 & (\Delta_{1,+}+\Delta_{1,-})^{-1}\Delta^{-1}_{1,+} & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & \cdots & (\Delta_{i,+}+\Delta_{i,-})^{-1}\Delta^{-1}_{i,-} & -\Delta^{-1}_{i,-}\Delta^{-1}_{i,+} & (\Delta_{i,+}+\Delta_{i,-})^{-1}\Delta^{-1}_{i,+} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & (\Delta_{M,+}+\Delta_{M,-})^{-1}\Delta^{-1}_{M,-} & \Xi_M \end{pmatrix}_{M\times M} \tag{85}$$

$$I^B \equiv \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix}_{M\times M} \tag{86}$$

where

$$\Xi_1 = -2\left[\Delta^{-1}_{1,-}\Delta^{-1}_{1,+} + (-1+\underline{\xi}\Delta_{1,-})^{-1}(\Delta_{1,+}+\Delta_{1,-})^{-1}\Delta^{-1}_{1,-}\right] \tag{87}$$

$$\Xi_M = -2\left[\Delta^{-1}_{M,-}\Delta^{-1}_{M,+} - (1+\overline{\xi}\Delta_{M,+})^{-1}(\Delta_{M,+}+\Delta_{M,-})^{-1}\Delta^{-1}_{M,+}\right] \tag{88}$$

Or, alternatively, with vectorized differences:

$$L_{1-}^B \equiv \text{tridiag}\left[-(\Delta_-^\circ)^{-1}[2:M], \left(\Delta_{1,-}^{-1}[1+(-1+\underline{\xi}\Delta_{1,-})^{-1}]; (\Delta_-^\circ)^{-1}[2:M]\right), \mathbf{0}_{M-1}\right] \tag{89}$$

$$L_{1+}^B \equiv \text{tridiag}\left[\mathbf{0}_{M-1}, \left(-(\Delta_-^\circ)^{-1}[1:M-1]; \Delta_{M,+}^{-1}[-1+(1+\overline{\xi}\Delta_{M,+})^{-1}]\right), (\Delta_-^\circ)^{-1}[2:M]\right] \tag{90}$$

$$L_2^B \equiv 2\odot\text{tridiag}\Big[(\Delta_-^\circ+\Delta_+^\circ)^{-1}\odot(\Delta_-^\circ)^{-1}, \tag{91}$$

$$\left(\Xi_1; -(\Delta_-^\circ\odot\Delta_+^\circ)^{-1}[2:M-1]; \Xi_M\right), \tag{92}$$

$$(\Delta_-^\circ+\Delta_+^\circ)^{-1}\odot(\Delta_+^\circ)^{-1}\Big] \tag{93}$$

$$I^B \equiv \text{diag}(\mathbf{1}_M) \tag{94}$$

4.2.2 Absorbing barrier conditions

To apply an absorbing barrier condition $\tilde{v}(x_{\min}) = S$ for some $S \in \mathbb{R}$, with one reflecting barrier condition on the upper bound $v'(x_{\max}) = 0$, one can use

$$B = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 \end{bmatrix}_{2\times(M+2)} \qquad b = \begin{bmatrix} S \\ 0 \end{bmatrix} \tag{95}$$

Similarly, one can apply an absorbing condition on the upper bound $\tilde{v}(x_{\max}) = S$ for some $S \in \mathbb{R}$ and the

$$B = \begin{bmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 1 \end{bmatrix}_{2\times(M+2)} \qquad b = \begin{bmatrix} 0 \\ S \end{bmatrix} \tag{96}$$

Note that the corresponding B and b are identical with regular grid cases.

4.3 Examples

Examples 4.1. Consider $L = L_2$ to solve $Lv = f$ with $M = 3$ under uniform grids $\overline{x} = \{x_0, x_1, x_2, x_3, x_4\}$ and $\Delta = 1$, whose corresponding interior grid is $x = \{x_1, x_2, x_3\}$. This gives

$$L^B = \begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix} \tag{97}$$

so $L^B v = f$ on the grid x results in the following system

$$\begin{bmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} \tilde{v}(x_1) \\ \tilde{v}(x_2) \\ \tilde{v}(x_3) \end{bmatrix} = \begin{bmatrix} \tilde{f}(x_1) \\ \tilde{f}(x_2) \\ \tilde{f}(x_3) \end{bmatrix} \tag{98}$$

For the extended system we have

$$L = \begin{bmatrix} 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \end{bmatrix} \tag{99}$$

$$B = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \tag{100}$$

Constructing the stacked extended system (42) gives

$$\begin{bmatrix} 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} \tilde{v}(x_0) \\ \tilde{v}(x_1) \\ \tilde{v}(x_2) \\ \tilde{v}(x_3) \\ \tilde{v}(x_4) \end{bmatrix} = \begin{bmatrix} \tilde{f}(x_1) \\ \tilde{f}(x_2) \\ \tilde{f}(x_3) \\ 0 \\ 0 \end{bmatrix} \tag{101}$$

Note that substracting the first row of L by (-1) times the first row of B returns an identical system as (101). Likewise, substracting the last row of L by (-1) times the last row of B returns the identical system. Performing the two Gaussian elimination yields the following system:

$$\begin{bmatrix} 0 & -1 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} \tilde{v}(x_0) \\ \tilde{v}(x_1) \\ \tilde{v}(x_2) \\ \tilde{v}(x_3) \\ \tilde{v}(x_4) \end{bmatrix} = \begin{bmatrix} \tilde{f}(x_2) \\ \tilde{f}(x_3) \\ \tilde{f}(x_4) \\ 0 \\ 0 \end{bmatrix} \tag{102}$$

Note that now we have the first three rows of the coefficient matrix with zero columns on the extended nodes, $\tilde{v}(x_1 - \Delta)$ and $\tilde{v}(x_3 + \Delta)$. Extracting the system corresponding to the first three rows returns the following system, which solves the interior of $\bar{v}$, i.e., v:

$$\begin{bmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} \tilde{v}(x_1) \\ \tilde{v}(x_2) \\ \tilde{v}(x_3) \end{bmatrix} = \begin{bmatrix} \tilde{f}(x_1) \\ \tilde{f}(x_2) \\ \tilde{f}(x_3) \end{bmatrix} \tag{103}$$

which is identical as (98).

Examples 4.2. Consider solving (98), but this time with an absorbing barrier condition on the lower bound, $\tilde{v}(x_{\min}) = S$ with a boundary condition matrix

$$B = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \tag{104}$$

The corresponding extended system is

$$\begin{bmatrix} 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} \tilde{v}(x_0) \\ \tilde{v}(x_1) \\ \tilde{v}(x_2) \\ \tilde{v}(x_3) \\ \tilde{v}(x_4) \end{bmatrix} = \begin{bmatrix} \tilde{f}(x_1) \\ \tilde{f}(x_2) \\ \tilde{f}(x_3) \\ S \\ 0 \end{bmatrix} \tag{105}$$

Note that substracting the first row of L by (-1) times the first row of B returns an identical system as (105). Likewise, substracting the last row of L by (-1) times the last row of B returns the identical system. Performing the two Gaussian elimination yields the following system:

$$\begin{bmatrix} 0 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} \tilde{v}(x_0) \\ \tilde{v}(x_1) \\ \tilde{v}(x_2) \\ \tilde{v}(x_3) \\ \tilde{v}(x_4) \end{bmatrix} = \begin{bmatrix} \tilde{f}(x_1) - S \\ \tilde{f}(x_2) \\ \tilde{f}(x_3) \\ 0 \\ 0 \end{bmatrix} \tag{106}$$

Extracting the system corresponding to the first three rows returns the following system, which solves the interior of $\bar{v}$, i.e., v:

$$\begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} \tilde{v}(x_1) \\ \tilde{v}(x_2) \\ \tilde{v}(x_3) \end{bmatrix} = \begin{bmatrix} \tilde{f}(x_1) - S \\ \tilde{f}(x_2) \\ \tilde{f}(x_3) \end{bmatrix} \tag{107}$$

A Derivation by substitution

One can also derive the formula for $L^B_{1-}, L^B_{1+}, L^B_2$ in (54), (55), (56) by substitution. For simplicity, here we focus on the case when we have regular grids, i.e., $x_{i+1} - x_i = \Delta$ for some $\Delta > 0$ for all $i = 0, ..., M$.

Using the backwards first-order difference, (13) implies

$$\frac{\tilde{v}(x_1) - \tilde{v}(x_0)}{\Delta} = -\underline{\xi}\tilde{v}(x_0) \tag{108}$$

i.e.,

$$\tilde{v}(x_0) = \frac{1}{1 - \underline{\xi}\Delta}\tilde{v}(x_1) \tag{109}$$

at the lower bound.

Likewise, (14) under the forwards first-order difference yields

$$\frac{\tilde{v}(x_{M+1}) - \tilde{v}(x_M)}{\Delta} = -\overline{\xi}\tilde{v}(x_{M+1}) \tag{110}$$

i.e.,

$$\tilde{v}(x_{M+1}) = \frac{1}{1 + \overline{\xi}\Delta}\tilde{v}(x_M) \tag{111}$$

at the upper bound.

The discretized central difference of second order under (13) at the lower bound is, by substituting (109) in,

$$\begin{aligned}
\frac{\tilde{v}(x_1 + \Delta) - 2\tilde{v}(x_1) + \tilde{v}(x_{\min})}{\Delta^2} &= \frac{\tilde{v}(x_1 + \Delta) - \tilde{v}(x_1)}{\Delta^2} - \frac{1}{\Delta}\frac{\tilde{v}(x_1) - \tilde{v}(x_{\min})}{\Delta} && (112)\\
&= \frac{\tilde{v}(x_1 + \Delta) - \tilde{v}(x_1)}{\Delta^2} + \frac{1}{\Delta}\underline{\xi}\tilde{v}(x_1) && (113)\\
&= \frac{1}{\Delta^2}(-1 + \Delta\underline{\xi})^{-1}\tilde{v}(x_1) + \frac{1}{\Delta^2}\tilde{v}(x_1 + \Delta) && (114)
\end{aligned}$$

Similarly, by (14), we have

$$\begin{aligned}
\frac{\tilde{v}(x_{\max}) - 2\tilde{v}(x_M) + \tilde{v}(x_M - \Delta)}{\Delta^2} &= \frac{\tilde{v}(x_M - \Delta) - \tilde{v}(x_M)}{\Delta^2} + \frac{1}{\Delta}\frac{\tilde{v}(x_{\max}) - \tilde{v}(x_M)}{\Delta} && (115)\\
&= \frac{\tilde{v}(x_M - \Delta) - \tilde{v}(x_M)}{\Delta^2} - \frac{1}{\Delta}\overline{\xi}\tilde{v}(x_M) && (116)\\
&= \frac{1}{\Delta^2}(-1 - \Delta\overline{\xi})^{-1}\tilde{v}(x_M) + \frac{1}{\Delta^2}\tilde{v}(x_M - \Delta) && (117)
\end{aligned}$$

at the upper bound.

Thus, the corresponding discretized differential operator L_{1-}, L_{1+}, and L_2 are defined as

$$L_{1-}^B \equiv \frac{1}{\Delta}\begin{pmatrix} 1-(1-\underline{\xi}\Delta)^{-1} & 0 & 0 & \dots & 0 & 0 & 0 \\ -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -1 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{pmatrix}_{M\times M} \tag{118}$$

$$L_{1+}^B \equiv \frac{1}{\Delta}\begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & -1+(1-\overline{\xi}\Delta)^{-1} \end{pmatrix}_{M\times M} \tag{119}$$

$$L_{2}^B \equiv \frac{1}{\Delta^2}\begin{pmatrix} -2-(1-\underline{\xi}\Delta)^{-1} & 1 & 0 & \dots & 0 & 0 & 0 \\ 1 & -2 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & -2 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -2+(1+\overline{\xi}\Delta)^{-1} \end{pmatrix}_{M\times M} \tag{120}$$