Derivations, extensions, and applications for `SimpleDifferentialOperators.jl`

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1 Setup

- Define an irregular grid $\{x_i\}_{i=1}^M$ with $x_1 = x_{\min}$ and $x_M = x_{\max}$. Denote the grid with the variable name, i.e. $x \equiv \{x_i\}_{i=1}^M$.
- Denote the distance between the grid points as

$$\Delta_{i,-} \equiv x_i - x_{i-1}, \text{ for } i = 2, \dots, M \tag{1}$$
$$\Delta_{i,+} \equiv x_{i+1} - x_i, \text{ for } i = 1, \dots, M-1 \tag{2}$$

- Assume $\Delta_{1,-} = \Delta_{1,+}$ and $\Delta_{M,+} = \Delta_{M,-}$, due to ghost points, x_0 and x_{M+1} on both boundaries. (i.e. the distance to the ghost nodes are the same as the distance to the closest nodes). Then define the vector of backwards and forwards first differences as

$$\Delta_- \equiv \begin{bmatrix} \Delta_{1,-} \\ \text{diff}(x) \end{bmatrix} \tag{3}$$
$$\Delta_+ \equiv \begin{bmatrix} \text{diff}(x) \\ \Delta_{M,+} \end{bmatrix} \tag{4}$$

- Reflecting barrier conditions:

$$\underline{\xi} v(x_{\min}) + \boldsymbol{\partial}_x v(x_{\min}) = 0 \tag{5}$$
$$\overline{\xi} v(x_{\max}) + \boldsymbol{\partial}_x v(x_{\max}) = 0 \tag{6}$$

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 (5) and (6), such that $L_{1-}v(x), L_{1+}v(x)$ and $L_2 v(x)$ represent the first-order (backward and forward) and second-order derivatives of $v(x)$ respectively at x. For second derivatives, we use the following numerical scheme from **?**:

$$v''(x_i) \approx \frac{\Delta_{i,-} v(x_i + \Delta_{i,+}) - (\Delta_{i,+} + \Delta_{i,-}) v(x_i) + \Delta_{i,+} v(x_i - \Delta_{i,-})}{\frac{1}{2}(\Delta_{i,+} + \Delta_{i,-})\Delta_{i,+}\Delta_{i,-}}, \text{for } i = 1, \dots, M \tag{7}$$

1.1 Regular grids

Suppose that the grids are regular, i.e., elements of $\text{diff}(x)$ are all identical with Δ for some $\Delta > 0$.

Using the backwards first-order difference, (5) implies

$$\frac{v(x_{\min}) - v(x_{\min} - \Delta)}{\Delta} = -\underline{\xi} v(x_{\min}) \tag{8}$$

at the lower bound.

Likewise, (6) under the forwards first-order difference yields

$$\frac{v(x_{\max} + \Delta) - v(x_{\max})}{\Delta} = -\overline{\xi} v(x_{\max}) \tag{9}$$

at the upper bound.

The discretized central difference of second order under (5) at the lower bound is

$$\frac{v(x_{\min} + \Delta) - 2v(x_{\min}) + v(x_{\min} - \Delta)}{\Delta^2} = \frac{v(x_{\min} + \Delta) - v(x_{\min})}{\Delta^2} - \frac{1}{\Delta}\frac{v(x_{\min}) - v(x_{\min} - \Delta)}{\Delta} \tag{10}$$

$$= \frac{v(x_{\min} + \Delta) - v(x_{\min})}{\Delta^2} + \frac{1}{\Delta}\underline{\xi} v(x_{\min}) \tag{11}$$

$$= \frac{1}{\Delta^2}(-1 + \Delta\underline{\xi}) v(x_{\min}) + \frac{1}{\Delta^2} v(x_{\min} + \Delta) \tag{12}$$

Similarly, by (6), we have

$$\frac{v(x_{\max} + \Delta) - 2v(x_{\max}) + v(x_{\max} - \Delta)}{\Delta^2} = \frac{v(x_{\max} - \Delta) - v(x_{\max})}{\Delta^2} + \frac{1}{\Delta}\frac{v(x_{\max} + \Delta) - v(x_{\max})}{\Delta} \tag{13}$$

$$= \frac{v(x_{\max} - \Delta) - v(x_{\max})}{\Delta^2} - \frac{1}{\Delta}\overline{\xi} v(x_{\max}) \tag{14}$$

$$= \frac{1}{\Delta^2}(-1 - \Delta\overline{\xi}) v(x_{\max}) + \frac{1}{\Delta^2} v(x_{\max} - \Delta) \tag{15}$$

at the upper bound.

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

$$L_{1-} \equiv \frac{1}{\Delta}\begin{pmatrix} 1 - (1 + \underline{\xi}\Delta) & 0 & 0 & \dots & 0 & 0 & 0 \\ -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -1 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{pmatrix}_{M\times M} \tag{16}$$

$$L_{1+} \equiv \frac{1}{\Delta}\begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & -1 + (1 - \overline{\xi}\Delta) \end{pmatrix}_{M\times M} \tag{17}$$

$$L_2 \equiv \frac{1}{\Delta^2}\begin{pmatrix} -2 + (1 + \underline{\xi}\Delta) & 1 & 0 & \dots & 0 & 0 & 0 \\ 1 & -2 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & -2 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -2 + (1 - \overline{\xi}\Delta) \end{pmatrix}_{M\times M} \tag{18}$$

1.2 Irregular grids

Using the backwards first-order difference, (5) implies

$$\frac{v(x_{\min}) - v(x_{\min} - \Delta_{1,-})}{\Delta_{1,-}} = -\underline{\xi} v(x_{\min}) \tag{19}$$

at the lower bound. Likewise, the forwards first-order difference under (6) yields

$$\frac{v(x_{\max} + \Delta_{M,+}) - v(x_{\max})}{\Delta_{M,+}} = -\overline{\xi} v(x_{\max}) \tag{20}$$

at the upper bound.

Note that we have assumed that $\Delta_{1,-} = \Delta_{1,+}$ and $\Delta_{M,+} = \Delta_{M,-}$ for the ghost notes. The discretized central difference of second order scheme at the lower bound under (5) is

$$\begin{aligned}
&\frac{\Delta_{1,-} v(x_{\min} + \Delta_{1,+}) - (\Delta_{1,+} + \Delta_{1,-}) v(x_{\min}) + \Delta_{1,+} v(x_{\min} - \Delta_{1,-})}{\frac{1}{2}(\Delta_{1,+} + \Delta_{1,-})\Delta_{1,+}\Delta_{1,-}} && (21)\\
&= \frac{v(x_{\min} + \Delta_{1,+}) - 2v(x_{\min}) + v(x_{\min} - \Delta_{1,+})}{\Delta_{1,+}^2} && (22)\\
&= \frac{v(x_{\min} + \Delta_{1,+}) - v(x_{\min})}{\Delta_{1,+}^2} - \frac{1}{\Delta_{1,+}} \frac{v(x_{\min}) - v(x_{\min} - \Delta_{1,+})}{\Delta_{1,+}} && (23)\\
&= \frac{v(x_{\min} + \Delta_{1,+}) - v(x_{\min})}{\Delta_{1,+}^2} + \frac{1}{\Delta_{i,+}} \underline{\xi} v(x_{\min}) && (24)\\
&= \frac{1}{\Delta_{1,+}^2}(-1 + \Delta_{1,+}\underline{\xi}) v(x_{\min}) + \frac{1}{\Delta_{1,+}^2} v(x_{\min} + \Delta_{1,+}) && (25)
\end{aligned}$$

Similarly, by (6), we have

$$\begin{aligned}
&\frac{\Delta_{M,-} v(x_{\max} + \Delta_{M,+}) - (\Delta_{M,+} + \Delta_{M,-}) v(x_{\max}) + \Delta_{M,+} v(x_{\max} - \Delta_{M,-})}{\frac{1}{2}(\Delta_{M,+} + \Delta_{M,-})\Delta_{M,+}\Delta_{M,-}} && (26)\\
&= \frac{v(x_{\max} + \Delta_{M,-}) - 2v(x_{\max}) + v(x_{\max} - \Delta_{M,-})}{\Delta_{M,-}^2} && (27)\\
&= \frac{v(x_{\max} - \Delta_{M,-}) - v(x_{\max})}{\Delta_{M,-}^2} + \frac{1}{\Delta_{M,-}} \frac{v(x_{\max} + \Delta_{M,-}) - v(x_{\max})}{\Delta_{M,-}} && (28)\\
&= \frac{v(x_{\max} - \Delta_{M,-}) - v(x_{\max})}{\Delta_{M,-}^2} - \frac{1}{\Delta_{M,-}} \overline{\xi} v(x_{\max}) && (29)\\
&= \frac{1}{\Delta_{M,-}^2}(-1 - \Delta_{M,-}\overline{\xi}) v(x_{\max}) + \frac{1}{\Delta_{M,-}^2} v(x_{\max} - \Delta_{M,-}) && (30)
\end{aligned}$$

at the upper bound.

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

$$L_{1-} \equiv \begin{pmatrix} \Delta_{1,-}^{-1}[1-(1+\underline{\xi}\Delta_{1,-})] & 0 & 0 & \dots & 0 & 0 & 0 \\ -\Delta_{2,-}^{-1} & \Delta_{2,-}^{-1} & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -\Delta_{M-1,-}^{-1} & \Delta_{M-1,-}^{-1} & 0 \\ 0 & 0 & 0 & \cdots & 0 & -\Delta_{M,-}^{-1} & \Delta_{M,-}^{-1} \end{pmatrix}_{M\times M} \tag{31}$$

$$L_{1+} \equiv \begin{pmatrix} -\Delta_{1,+}^{-1} & \Delta_{1,+}^{-1} & 0 & \dots & 0 & 0 & 0 \\ 0 & -\Delta_{2,+}^{-1} & \Delta_{2,+}^{-1} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & -\Delta_{M-1,+}^{-1} & \Delta_{M-1,+}^{-1} \\ 0 & 0 & 0 & \dots & 0 & 0 & \Delta_{M,+}^{-1}[-1+(1-\overline{\xi}\Delta_{M,+})] \end{pmatrix}_{M\times M} \tag{32}$$

$$L_2 \equiv \begin{pmatrix} \Delta_{1,+}^{-2}[-2+(1+\underline{\xi}\Delta_{1,+})] & \Delta_{1,+}^{-2} & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & \cdots & 2(\Delta_{i,+}+\Delta_{i,-})^{-1}\Delta_{i,-}^{-1} & -2\Delta_{i,-}^{-1}\Delta_{i,+}^{-1} & 2(\Delta_{i,+}+\Delta_{i,-})^{-1}\Delta_{i,+}^{-1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \Delta_{M,-}^{-2} & \Delta_{M,-}^{-2}[-2+(1-\overline{\xi}\Delta_{M,-})] \end{pmatrix}_{M\times M} \tag{33}$$

1.3 Differential operators by basis

Define the following basis matrices:

$$U_1^- \equiv \begin{pmatrix} 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -1 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{pmatrix}_{M\times M} \tag{34}$$

$$U_1^+ \equiv \begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & -1 \end{pmatrix}_{M\times M} \tag{35}$$

$$\tag{36}$$

and the boundary conditions for the reflecting conditions:

$$B_1 \equiv \begin{pmatrix} (1+\underline{\xi}\Delta_{1,-}^{-1}) & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}_{M\times M} \tag{37}$$

$$B_M \equiv \begin{pmatrix} 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & (1-\overline{\xi}\Delta_{M,+}^{-1}) \end{pmatrix}_{M\times M} \tag{38}$$

1.3.1 Regular grids

For regular grids with the uniform distance of $\Delta > 0$, (16) and (18) can be represented by

$$L_{1-} = \frac{1}{\Delta}U_1^- - B_1 \tag{39}$$

$$L_{1+} = \frac{1}{\Delta}U_1^+ + B_M \tag{40}$$

$$L_2 = \frac{1}{\Delta^2}(U_1^+ - U_1^-) + B_1 + B_M \tag{41}$$

1.3.2 Irregular grids

For notational brevity, for vectors with the same size, x_1, x_2, define x_1x_2 as the elementwise-multiplied vector. Then, we have

$$L_{1-} = \mathrm{diag}(\Delta_-)^{-1}U_1^- - B_1 \tag{42}$$

$$L_{1+} = \mathrm{diag}(\Delta_+)^{-1}U_1^+ + B_M \tag{43}$$

$$L_2 = \mathrm{diag}\left[\frac{1}{2}(\Delta_+ + \Delta_-)\Delta_+\right]^{-1} U_1^+ - \mathrm{diag}\left[\frac{1}{2}(\Delta_+ + \Delta_-)\Delta_-\right]^{-1} U_1^- + B_1 + B_M \tag{44}$$

We can simplify this expression further by introducing a new notation. Let x^{-1} be defined as the elementwise inverse of a vector x that contains no zero element. Then, L_2 can be represented as

$$\begin{aligned} L_2 &= 2\left[\mathrm{diag}\left((\Delta_+ + \Delta_-)^{-1}\Delta_+^{-1}\right)U_1^+ - \mathrm{diag}\left((\Delta_+ + \Delta_-)^{-1}\Delta_-^{-1}\right)U_1^-\right] + B_1 + B_M && (45) \\ &= 2\mathrm{diag}\left((\Delta_+ + \Delta_-)^{-1}\right)\left[\mathrm{diag}\left(\Delta_+^{-1}\right)U_1^+ - \mathrm{diag}\left(\Delta_-^{-1}\right)U_1^-\right] + B_1 + B_M && (46) \end{aligned}$$

The diagonal elements of (46) are also identical with the one provided in (33) – to see this, note that the diagonal elements of (46), modulo B_1 and B_M, are

$$\begin{aligned} -2\left[(\Delta_+ + \Delta_-)^{-1}\Delta_+^{-1} + (\Delta_+ + \Delta_-)^{-1}\Delta_-^{-1}\right] &= -2(\Delta_+ + \Delta_-)^{-1}(\Delta_+^{-1} + \Delta_-^{-1}) && (47) \\ &= -2(\Delta_+ + \Delta_-)^{-1}(\Delta_+^{-1}\Delta_-^{-1})(\Delta_+ + \Delta_-) && (48) \\ &= -2(\Delta_+^{-1}\Delta_-^{-1}) && (49) \end{aligned}$$

which is identical with $\mathrm{diag}(L_2)$ with L_2 from (33) except the first row and last row that are affected by B_1 and B_M.

2 Boundary conditions with operators on extended grids

Boundary conditions can be applied manually by using operators on extended grids. This can be done by first extending $x = \{x_i\}_{i=1}^{M}$ to $\overline{x} = \{x_i\}_{i=0}^{M+1}$ such that $x_1 - x_0 = \Delta_{1,+} (= \Delta_{1,-})$ and $x_{M+1} - x_M = \Delta_{M,-} (= \Delta_{M,+})$. We call x_0 and x_{M+1}, the extra nodes just before and after $x_{\min}$ and $x_{\max}$, as ghost nodes. Likewise, define $v(\overline{x})$ as $(M+2)$-vector whose ith element is $\overline{x}_i$. We can then define the following operators on $\overline{x}$:

$$\overline{L}_{1-} \equiv \begin{pmatrix} -\Delta_{1,-}^{-1} & \Delta_{1,-}^{-1} & 0 & \dots & 0 & 0 & 0 \\ 0 & -\Delta_{2,-}^{-1} & \Delta_{2,-}^{-1} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \Delta_{M-1,-}^{-1} & 0 & 0 \\ 0 & 0 & 0 & \cdots & -\Delta_{M,-}^{-1} & \Delta_{M,-}^{-1} & 0 \end{pmatrix}_{M \times (M+2)} \tag{50}$$

$$\overline{L}_{1+} \equiv \begin{pmatrix} 0 & -\Delta_{1,+}^{-1} & \Delta_{1,+}^{-1} & \dots & 0 & 0 & 0 \\ 0 & 0 & -\Delta_{2,+}^{-1} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -\Delta_{M-1,+}^{-1} & \Delta_{M-1,+}^{-1} & 0 \\ 0 & 0 & 0 & \cdots & 0 & -\Delta_{M,+}^{-1} & \Delta_{M,+}^{-1} \end{pmatrix}_{M \times (M+2)} \tag{51}$$

$$\overline{L}_2 \equiv \frac{1}{\Delta^2} \begin{pmatrix} \Delta_{1,-}^{-2} & -2\Delta_{1,-}^{-1}\Delta_{1,+}^{-1} & \Delta_{i,+}^{-2} & \dots & 0 & 0 & 0 \\ 0 & 2(\Delta_{2,+}+\Delta_{2,-})^{-1}\Delta_{2,-}^{-1} & -2\Delta_{2,-}^{-1}\Delta_{2,+}^{-1} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -2\Delta_{M-1,-}^{-1}\Delta_{M-1,+}^{-1} & 2(\Delta_{M-1,+}+\Delta_{M-1,-})^{-1}\Delta_{M-1,+}^{-1} & 0 \\ 0 & 0 & 0 & \dots & \Delta_{M,-}^{-2} & -2\Delta_{M,-}^{-1}\Delta_{M,+}^{-1} & \Delta_{M,+}^{-2} \end{pmatrix}_{M \times (M+2)} \tag{52}$$

Suppose that we want to solve a system $Lv(x) = f(x)$ for $v(x)$ where L is a linear combination of discretized differential operators for some $f(x)$ that represents the values of a function f on discretized x. To solve the system under boundary conditions on v, one can construct and solve the following extended system:

$$\begin{bmatrix} \overline{L} \\ B \end{bmatrix} v(\overline{x}) = \begin{bmatrix} f(x) \\ b \end{bmatrix} \tag{53}$$

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.

2.1 Reflecting barrier conditions

To apply reflecting barrier conditions $v'(x_{\min}) = v'(x_{\max}) = 0$, one can use

$$B = \begin{bmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 \end{bmatrix}_{2 \times (M+2)} \qquad b = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{54}$$

2.1.1 Gaussian elimination

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

Examples 2.1. Consider $L = L_2$ to solve $Lv = f(x)$ with $M = 3$ under uniform grids $x = \{x_2, x_3, x_4\}$ and $\Delta = 1$, whose corresponding extended grid is $\{x_1, x_2, x_3, x_4, x_5\}$. This gives

$$L = \begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix} \tag{55}$$

so $Lv = f(x)$ on the grid x results in the following system

$$\begin{bmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} v(x_2) \\ v(x_3) \\ v(x_4) \end{bmatrix} = \begin{bmatrix} f(x_2) \\ f(x_3) \\ f(x_4) \end{bmatrix} \tag{56}$$

For the extended system we have

$$\overline{L} = \begin{bmatrix} 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \end{bmatrix} \tag{57}$$

$$B = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \tag{58}$$

Constructing the stacked extended system (**??**) gives

$$\begin{bmatrix} 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} v(x_1) \\ v(x_2) \\ v(x_3) \\ v(x_4) \\ v(x_5) \end{bmatrix} = \begin{bmatrix} f(x_2) \\ f(x_3) \\ f(x_4) \\ 0 \\ 0 \end{bmatrix} \tag{59}$$

Note that substracting the first row of $\overline{L}$ by (-1) times the first row of B returns an identical system as (**??**). Likewise, substracting the last row of $\overline{L}$ by (-1) times the last row of B returns the identical system. Performing the two Gaussian elimination yields the following system:

$$\begin{bmatrix} 0 & -1 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} v(x_1) \\ v(x_2) \\ v(x_3) \\ v(x_4) \\ v(x_5) \end{bmatrix} = \begin{bmatrix} f(x_2) \\ f(x_3) \\ f(x_4) \\ 0 \\ 0 \end{bmatrix} \tag{60}$$

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

$$\begin{bmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} v(x_2) \\ v(x_3) \\ v(x_4) \end{bmatrix} = \begin{bmatrix} f(x_2) \\ f(x_3) \\ f(x_4) \end{bmatrix} \tag{61}$$

which is identical as (**??**).

2.2 Absorbing barrier conditions

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

$$B = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 \end{bmatrix}_{2\times(M+2)} \qquad b = \begin{bmatrix} S \\ 0 \end{bmatrix} \tag{62}$$

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

$$B = \begin{bmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 1 \end{bmatrix}_{2\times(M+2)} \qquad b = \begin{bmatrix} 0 \\ S \end{bmatrix} \tag{63}$$

2.2.1 Gaussian elimination

Examples 2.2. Consider solving (**??**), but this time with an absorbing barrier condition on the lower bound, $v(x_1 - \Delta) = S$ with a boundary condition matrix

$$B = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \tag{64}$$

The corresponding extended system is

$$\begin{bmatrix} 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} v(x_1 - \Delta) \\ v(x_1) \\ v(x_2) \\ v(x_3) \\ v(x_3 + \Delta) \end{bmatrix} = \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ S \\ 0 \end{bmatrix} \tag{65}$$

Note that substracting the first row of $\overline{L}$ by (-1) times the first row of B returns an identical system as (**??**). Likewise, substracting the last row of $\overline{L}$ by (-1) times the last row of B returns the identical system. Performing the two Gaussian elimination yields the following system:

$$\begin{bmatrix} 0 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} v(x_1 - \Delta) \\ v(x_1) \\ v(x_2) \\ v(x_3) \\ v(x_3 + \Delta) \end{bmatrix} = \begin{bmatrix} f(x_1) - S \\ f(x_2) \\ f(x_3) \\ 0 \\ 0 \end{bmatrix} \tag{66}$$

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

$$\begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} v(x_1) \\ v(x_2) \\ v(x_3) \end{bmatrix} = \begin{bmatrix} f(x_1) - S \\ f(x_2) \\ f(x_3) \end{bmatrix} \tag{67}$$

3 Applications

3.1 Hamilton–Jacobi–Bellman equations (HJBE)

Consider solving for v from the following optimal control problem

$$v(x_0) = \max_{\{\alpha(t)\}_{t\geq 0}} \int_0^\infty e^{-\rho t} r(x(t), \alpha(t)) dt \tag{68}$$

with the law of motion for the state

$$dx = \mu dt + \sigma dW \tag{69}$$

for some constant $\mu \geq 0$ and $\sigma \geq 0$ with $x(0) = x_0$.

Let $\alpha^*(t)$ be the optimal solution. Suppose that r under $\alpha^*(t)$ can be expressed in terms of state variables, $r^*(x)$. Then, the HJBE yields

$$\rho v(x) = r^*(x) + \mu \partial_x v(x) + \frac{\sigma^2}{2} \partial_{xx} v(x) \tag{70}$$

In terms of differential operators, one can rewrite the equation as

$$\tilde{L} v(x) = r^*(x) \tag{71}$$

with $\tilde{L} = \rho - \tilde{L}_x$ where $\tilde{L}_x$ is defined as

$$\tilde{L}_x = \mu \partial_x + (\sigma^2/2) \partial_{xx} \tag{72}$$

By descretizing the space of x, one can solve the corresponding system by using discretized operators for ∂_x (L_{1+}), ∂_{xx} (L_2) on some grids of length M, $\{x_i\}_{i=1}^M$:

$$L_x = \mu L_{1+} + \frac{\sigma^2}{2} L_2 \tag{73}$$

so that v from (59) can be computed by solving the following discretized system of equations:

$$Lv = r^* \tag{74}$$

where v and r^* are M-vectors whose ith elements are $v(x_i)$ and $r^*(x_i)$, respectively, and L is defined as $L = \rho I - L_x$.

3.2 Kolmogorov forward equations (KFE) under diffusion process

Let $g(x,t)$ be the distribution of x at time t from the example above. By the Kolmogorov forward equation, the following PDE holds:

$$\partial_t g(x,t) = -\mu \partial_x g(x,t) + \frac{\sigma^2}{2} \partial_{xx} g(x,t) \tag{75}$$

3.2.1 Stationary distributions

The stationary distribution $g^*(x)$ satisfies

$$0 = -\mu \partial_x g^*(x) + \frac{\sigma^2}{2} \partial_{xx} g^*(x) \tag{76}$$

which can be rewritten as

$$\tilde{L}_x^* g(x) = 0 \tag{77}$$

where

$$\tilde{L}_x^* = -\mu \partial_x + (\sigma^2/2) \partial_{xx} \tag{78}$$

By descretizing the space of x, one can solve the corresponding system by using discretized operators for $\tilde{L}_x^*$. Note that the operator for the KFE in (66) is the adjoint operator of the operator for the HJBE in (60), and the correct discretization scheme for (66) can be, analogously, done by taking the transpose of the discretized operator for HJBE in (61) – see **?** and **?**. Hence, one can find the stationary distribution by solving the following discretized system of equations:

$$L_x^T g = 0 \tag{79}$$

where L_x^T is the transpose of L_x from (61) and g is an M-vector whose element is $g(x_i)$ such that $\sum_{i=1}^M g(x_i) = 1$.

3.2.2 Full dynamics of distributions

One can also solve the full PDE in (63), given an initial distribution $g(x, 0)$. After discretization, note that (63) can be rewritten as

$$\dot{g}(t) = L_x^T g(t) \tag{80}$$

where $\dot{g}(t)$ is an M-vector whose ith element is $\partial_t g(x_i, t)$, which can be efficently solved by a number of differential equation solvers available in public, including **?**.