Derivation on discretized differential operators on (ir)regular grids with boundary conditions

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1 Setup

- Define an irregular grid $\{z_i\}_{i=1}^P$ with $z_1 = \underline{z}$ and $z_P = \overline{z}$. Denote the grid with the variable name, i.e. $z \equiv \{z_i\}_{i=1}^P$.
- Denote the distance between the grid points as the *backwards* difference

$$\Delta_{i,-} \equiv z_i - z_{i-1}, \text{ for } i = 2, \dots, P \tag{1}$$

$$\Delta_{i,+} \equiv z_{i+1} - z_i, \text{ for } i = 1, \dots, P-1 \tag{2}$$

- Assume $\Delta_{1,-} = \Delta_{1,+}$ and $\Delta_{P,+} = \Delta_{P,-}$, due to ghost points, z_0 and z_{P+1} on both boundaries. (i.e.he 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

$$\Delta_- \equiv \begin{bmatrix} z_2 - z_1 \\ \text{diff}(z) \end{bmatrix} \tag{3}$$

$$\Delta_+ \equiv \begin{bmatrix} \text{diff}(z) \\ z_P - z_{P-1} \end{bmatrix} \tag{4}$$

- Reflecting barrier conditions:

$$\underline{\xi} v(\underline{z}) + \boldsymbol{\partial}_z v(\underline{z}) = 0 \tag{5}$$

$$\overline{\xi} v(\overline{z}) + \boldsymbol{\partial}_z v(\overline{z}) = 0 \tag{6}$$

Let L_1^- be the discretized backwards first differences and L_2 be the discretized central differences subject to the Neumann boundary conditions in **????** such that $L_1^- v(z)$ and $L_2 v(z)$ represent the first and second derivatives of $v(z)$ respectively at z. For second derivatives, we use the following numerical scheme from **?**:

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

1.1 Regular grids

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

Using the backwards first-order difference, (**??**) implies

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

at the lower bound.

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

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

at the upper bound.

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

$$\begin{aligned}\frac{v(\underline{z}+\Delta)-2v(\underline{z})+v(\underline{z}-\Delta)}{\Delta^2} &= \frac{v(\underline{z}+\Delta)-v(\underline{z})}{\Delta^2}-\frac{1}{\Delta}\frac{v(\underline{z})-v(\underline{z}-\Delta)}{\Delta} && (10)\\ &= \frac{v(\underline{z}+\Delta)-v(\underline{z})}{\Delta^2}+\frac{1}{\Delta}\underline{\xi}v(\underline{z}) && (11)\\ &= \frac{1}{\Delta^2}(-1+\Delta\underline{\xi})v(\underline{z})+\frac{1}{\Delta^2}v(\underline{z}+\Delta) && (12)\end{aligned}$$

Similarly, by (??), we have

$$\begin{aligned}\frac{v(\overline{z}+\Delta)-2v(\overline{z})+v(\overline{z}-\Delta)}{\Delta^2} &= \frac{v(\overline{z}-\Delta)-v(\overline{z})}{\Delta^2}+\frac{1}{\Delta}\frac{v(\overline{z}+\Delta)-v(\overline{z})}{\Delta} && (13)\\ &= \frac{v(\overline{z}-\Delta)-v(\overline{z})}{\Delta^2}-\frac{1}{\Delta}\overline{\xi}v(\overline{z}) && (14)\\ &= \frac{1}{\Delta^2}(-1-\Delta\overline{\xi})v(\overline{z})+\frac{1}{\Delta^2}v(\overline{z}-\Delta) && (15)\end{aligned}$$

at the upper bound.

Thus, the corresponding discretized differential operator L_1^-, L_1^+, and L_2 are defined as

$$L_1^- \equiv \frac{1}{\Delta}\begin{pmatrix} 1-(1+\underline{\xi}\Delta) & 0 & 0 & \dots & 0 & 0 & 0\\ -1 & 1 & 0 & \dots & 0 & 0 & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & \dots & -1 & 1 & 0\\ 0 & 0 & 0 & \cdots & 0 & -1 & 1\end{pmatrix}_{P\times P} \tag{16}$$

$$L_1^+ \equiv \frac{1}{\Delta}\begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0\\ 0 & -1 & 1 & \dots & 0 & 0 & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & \dots & 0 & -1 & 1\\ 0 & 0 & 0 & \cdots & 0 & 0 & -1+(1-\overline{\xi}\Delta)\end{pmatrix}_{P\times P} \tag{17}$$

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

1.2 Irregular grids

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

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

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

$$\frac{v(\overline{z}+\Delta_{P,+})-v(\overline{z})}{\Delta_{P,+}} = -\overline{\xi}v(\overline{z}) \tag{20}$$

at the upper bound.

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

$$\frac{\Delta_{1,-}v(\underline{z}+\Delta_{1,+}) - (\Delta_{1,+}+\Delta_{1,-})v(\underline{z}) + \Delta_{1,+}v(\underline{z}-\Delta_{1,-})}{\frac{1}{2}(\Delta_{1,+}+\Delta_{1,-})\Delta_{1,+}\Delta_{1,-}} \tag{21}$$

$$= \frac{v(\underline{z}+\Delta_{1,+}) - 2v(\underline{z}) + v(\underline{z}-\Delta_{1,+})}{\Delta_{1,+}^2} \tag{22}$$

$$= \frac{v(\underline{z}+\Delta_{1,+}) - v(\underline{z})}{\Delta_{1,+}^2} - \frac{1}{\Delta_{1,+}}\frac{v(\underline{z}) - v(\underline{z}-\Delta_{1,+})}{\Delta_{1,+}} \tag{23}$$

$$= \frac{v(\underline{z}+\Delta_{1,+}) - v(\underline{z})}{\Delta_{1,+}^2} + \frac{1}{\Delta_{i,+}}\underline{\xi}v(\underline{z}) \tag{24}$$

$$= \frac{1}{\Delta_{1,+}^2}(-1+\Delta_{1,+}\underline{\xi})v(\underline{z}) + \frac{1}{\Delta_{1,+}^2}v(\underline{z}+\Delta_{1,+}) \tag{25}$$

Similarly, by (**??**), we have

$$\frac{\Delta_{P,-}v(\overline{z}+\Delta_{P,+}) - (\Delta_{P,+}+\Delta_{P,-})v(\overline{z}) + \Delta_{P,+}v(\overline{z}-\Delta_{P,-})}{\frac{1}{2}(\Delta_{P,+}+\Delta_{P,-})\Delta_{P,+}\Delta_{P,-}} \tag{26}$$

$$= \frac{v(\overline{z}+\Delta_{P,-}) - 2v(\overline{z}) + v(\overline{z}-\Delta_{P,-})}{\Delta_{P,-}^2} \tag{27}$$

$$= \frac{v(\overline{z}-\Delta_{P,-}) - v(\overline{z})}{\Delta_{P,-}^2} + \frac{1}{\Delta_{P,-}}\frac{v(\overline{z}+\Delta_{P,-}) - v(\overline{z})}{\Delta_{P,-}} \tag{28}$$

$$= \frac{v(\overline{z}-\Delta_{P,-}) - v(\overline{z})}{\Delta_{P,-}^2} - \frac{1}{\Delta_{P,-}}\overline{\xi}v(\overline{z}) \tag{29}$$

$$= \frac{1}{\Delta_{P,-}^2}(-1-\Delta_{P,-}\overline{\xi})v(\overline{z}) + \frac{1}{\Delta_{P,-}^2}v(\overline{z}-\Delta_{P,-}) \tag{30}$$

at the upper bound.

Thus, the corresponding discretized differential operator L_1^-, L_1^+, and L_2 are defined as

$$L_1^- \equiv \begin{pmatrix} \Delta_{1,-}^{-1}[1-(1+\underline{\xi}\Delta_{1,-})] & 0 & 0 & \dots & 0 & 0 & 0 \\ -\Delta_{2,-}^{-1} & \Delta_{2,-}^{-1} & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -\Delta_{P-1,-}^{-1} & \Delta_{P-1,-}^{-1} & 0 \\ 0 & 0 & 0 & \cdots & 0 & -\Delta_{P,-}^{-1} & \Delta_{P,-}^{-1} \end{pmatrix}_{P\times P} \tag{31}$$

$$L_1^- \equiv \begin{pmatrix} -\Delta_{1,+}^{-1} & \Delta_{1,+}^{-1} & 0 & \dots & 0 & 0 & 0 \\ 0 & -\Delta_{2,+}^{-1} & \Delta_{2,+}^{-1} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & -\Delta_{P-1,+}^{-1} & \Delta_{P-1,+}^{-1} \\ 0 & 0 & 0 & \dots & 0 & 0 & \Delta_{P,+}^{-1}[-1+(1-\overline{\xi}\Delta_{P,+})] \end{pmatrix}_{P\times P} \tag{32}$$

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

1.3 Differential operators by basis

Define the following basis matrices:

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

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

$$\tag{36}$$

and the boundary conditions for the reflecting conditions:

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

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

1.3.1 Regular grids

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

$$
L_1^- = \frac{1}{\Delta}U_1^- - B_1 \tag{39}
$$

$$
L_1^+ = \frac{1}{\Delta}U_1^+ + B_P \tag{40}
$$

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

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

$$
L_1^- = \mathrm{diag}(\Delta_-)^{-1}U_1^- - B_1 \tag{42}
$$

$$
L_1^+ = \mathrm{diag}(\Delta_+)^{-1}U_1^+ + B_P \tag{43}
$$

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

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

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

The diagonal elements of (**??**) are also identical with the one provided in (**??**) – to see this, note that the diagonal elements of (**??**), modulo B_1 and B_P, 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 (**??**) except the first row and last row that are affected by B_1 and B_P.