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

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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 the *backwards* difference

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

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

- 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.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

$$\Delta_- \equiv \begin{bmatrix} x_2 - x_1 \\ \text{diff}(x) \end{bmatrix} \tag{3}$$

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

- 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^- be the discretized backwards first differences and L_2 be the discretized central differences subject to the Neumann boundary conditions in (5) and (6) such that $L_1^- v(x)$ and $L_2 v(x)$ represent the first and second derivatives of $v(x)$ respectively at x. For second derivatives, we use the following numerical scheme from **?**:

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

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

$$\begin{align}
\frac{v(x_{\min}+\Delta)-2v(x_{\min})+v(x_{\min}-\Delta)}{\Delta^2} &= \frac{v(x_{\min}+\Delta)-v(x_{\min})}{\Delta^2}-\frac{1}{\Delta}\frac{v(x_{\min})-v(x_{\min}-\Delta)}{\Delta} \tag{10}\\
&= \frac{v(x_{\min}+\Delta)-v(x_{\min})}{\Delta^2}+\frac{1}{\Delta}\underline{\xi}v(x_{\min}) \tag{11}\\
&= \frac{1}{\Delta^2}(-1+\Delta\underline{\xi})v(x_{\min})+\frac{1}{\Delta^2}v(x_{\min}+\Delta) \tag{12}
\end{align}$$

Similarly, by (6), we have

$$\begin{align}
\frac{v(x_{\max}+\Delta)-2v(x_{\max})+v(x_{\max}-\Delta)}{\Delta^2} &= \frac{v(x_{\max}-\Delta)-v(x_{\max})}{\Delta^2}+\frac{1}{\Delta}\frac{v(x_{\max}+\Delta)-v(x_{\max})}{\Delta} \tag{13}\\
&= \frac{v(x_{\max}-\Delta)-v(x_{\max})}{\Delta^2}-\frac{1}{\Delta}\overline{\xi}v(x_{\max}) \tag{14}\\
&= \frac{1}{\Delta^2}(-1-\Delta\overline{\xi})v(x_{\max})+\frac{1}{\Delta^2}v(x_{\max}-\Delta) \tag{15}
\end{align}$$

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 $x_1 x_2$ as the elementwise-multiplied vector. Then, we have

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

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

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

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

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

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