

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

$$\Delta_{i,-} \equiv x_i - x_{i-1}, \text{ for } i = 2, \dots, M \quad (1)$$

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

- 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

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

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

- Reflecting barrier conditions:

$$\underline{\xi}v(x_{\min}) + \partial_x v(x_{\min}) = 0 \quad (5)$$

$$\bar{\xi}v(x_{\max}) + \partial_x v(x_{\max}) = 0 \quad (6)$$

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 ?:

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

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

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

at the lower bound.

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

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

at the upper bound.

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

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

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

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

Similarly, by (6), we have

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

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

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

at the upper bound.

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

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

$$L_1^+ \equiv \frac{1}{\Delta} \begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 \\ 0 & 0 & 0 & \dots & 0 & 0 & -1 + (1 - \bar{\xi}\Delta) \end{pmatrix}_{M \times M} \quad (17)$$

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

1.2 Irregular grids

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

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

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

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

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

$$\frac{\Delta_{1,-}v(x_{\min} + \Delta_{1,+}) - (\Delta_{1,+} + \Delta_{1,-})v(x_{\min}) + \Delta_{1,+}v(x_{\min} - \Delta_{1,-})}{\frac{1}{2}(\Delta_{1,+} + \Delta_{1,-})\Delta_{1,+}\Delta_{1,-}} \quad (21)$$

$$= \frac{v(x_{\min} + \Delta_{1,+}) - 2v(x_{\min}) + v(x_{\min} - \Delta_{1,+})}{\Delta_{1,+}^2} \quad (22)$$

$$= \frac{v(x_{\min} + \Delta_{1,+}) - v(x_{\min})}{\Delta_{1,+}^2} - \frac{1}{\Delta_{1,+}} \frac{v(x_{\min}) - v(x_{\min} - \Delta_{1,+})}{\Delta_{1,+}} \quad (23)$$

$$= \frac{v(x_{\min} + \Delta_{1,+}) - v(x_{\min})}{\Delta_{1,+}^2} + \frac{1}{\Delta_{1,+}} \bar{\xi}v(x_{\min}) \quad (24)$$

$$= \frac{1}{\Delta_{1,+}^2}(-1 + \Delta_{1,+}\bar{\xi})v(x_{\min}) + \frac{1}{\Delta_{1,+}^2}v(x_{\min} + \Delta_{1,+}) \quad (25)$$

Similarly, by (6), we have

$$\frac{\Delta_{M,-}v(x_{\max} + \Delta_{M,+}) - (\Delta_{M,+} + \Delta_{M,-})v(x_{\max}) + \Delta_{M,+}v(x_{\max} - \Delta_{M,-})}{\frac{1}{2}(\Delta_{M,+} + \Delta_{M,-})\Delta_{M,+}\Delta_{M,-}} \quad (26)$$

$$= \frac{v(x_{\max} + \Delta_{M,-}) - 2v(x_{\max}) + v(x_{\max} - \Delta_{M,-})}{\Delta_{M,-}^2} \quad (27)$$

$$= \frac{v(x_{\max} - \Delta_{M,-}) - v(x_{\max})}{\Delta_{M,-}^2} + \frac{1}{\Delta_{M,-}} \frac{v(x_{\max} + \Delta_{M,-}) - v(x_{\max})}{\Delta_{M,-}} \quad (28)$$

$$= \frac{v(x_{\max} - \Delta_{M,-}) - v(x_{\max})}{\Delta_{M,-}^2} - \frac{1}{\Delta_{M,-}} \bar{\xi}v(x_{\max}) \quad (29)$$

$$= \frac{1}{\Delta_{M,-}^2}(-1 - \Delta_{M,-}\bar{\xi})v(x_{\max}) + \frac{1}{\Delta_{M,-}^2}v(x_{\max} - \Delta_{M,-}) \quad (30)$$

at the upper bound.

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

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

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

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

1.3 Differential operators by basis

Define the following basis matrices:

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

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

$$(36)$$

and the boundary conditions for the reflecting conditions:

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

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

1.3.1 Regular grids

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

$$L_1^- = \frac{1}{\Delta} U_1^- - B_1 \quad (39)$$

$$L_1^+ = \frac{1}{\Delta} U_1^+ + B_M \quad (40)$$

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

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

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

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

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

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

$$L_2 = 2 \left[\text{diag} \left((\Delta_+ + \Delta_-)^{-1} \Delta_+^{-1} \right) U_1^+ - \text{diag} \left((\Delta_+ + \Delta_-)^{-1} \Delta_-^{-1} \right) U_1^- \right] + B_1 + B_M \quad (45)$$

$$= 2 \text{diag} \left((\Delta_+ + \Delta_-)^{-1} \right) \left[\text{diag} \left(\Delta_+^{-1} \right) U_1^+ - \text{diag} \left(\Delta_-^{-1} \right) U_1^- \right] + B_1 + B_M \quad (46)$$

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

$$-2 \left[(\Delta_+ + \Delta_-)^{-1} \Delta_+^{-1} + (\Delta_+ + \Delta_-)^{-1} \Delta_-^{-1} \right] = -2 (\Delta_+ + \Delta_-)^{-1} (\Delta_+^{-1} + \Delta_-^{-1}) \quad (47)$$

$$= -2 (\Delta_+ + \Delta_-)^{-1} (\Delta_+^{-1} \Delta_-^{-1}) (\Delta_+ + \Delta_-) \quad (48)$$

$$= -2 (\Delta_+^{-1} \Delta_-^{-1}) \quad (49)$$

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