

# 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) 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 [1]:

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

### 1.1 Regular grids

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

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

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

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

### 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  $\Delta > 0$ , (??) and (??) 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 (??) are also identical with the one provided in (??) – to see this, note that the diagonal elements of (??), 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 (??) except the first row and last row that are affected by  $B_1$  and  $B_M$ .