

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

February 14, 2019

1 Setup

- Define an irregular grid $\{z_i\}_{i=1}^P$ with $z_1 = \underline{z}$ and $z_P = \bar{z}$. 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

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

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

- 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. 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

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

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

- Reflecting barrier conditions:

$$\xi v(\underline{z}) + \partial_z v(\underline{z}) = 0 \quad (5)$$

$$\xi v(\bar{z}) + \partial_z v(\bar{z}) = 0 \quad (6)$$

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 $L_1^- v(z)$ 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 Achdou et al. (2017):

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

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, (5) implies

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

at the lower bound.

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

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

at the upper bound.

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

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

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

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

Similarly, by (6), we have

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

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

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

at the upper bound.

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

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

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

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

1.2 Irregular grids

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

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

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

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

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 (5) is

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

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

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

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

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

Similarly, by (6), we have

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

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

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

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

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

at the upper bound.

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

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

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

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

1.3 Differential operators by basis

Define the following basis matrices:

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

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

$$(36)$$

and the boundary conditions for the reflecting conditions:

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

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

1.3.1 Regular grids

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

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

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

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

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

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

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

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

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

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

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

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_P , 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_P .

References

Achdou Y., Han J., Lasry J.-M., Lions P.-L., Moll B., 2017, Technical report, Income and wealth distribution in macroeconomics: A continuous-time approach. National Bureau of Economic Research