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

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1 Setup

- Define an irregular grid $\{z_i\}_{i=1}^M$ with $z_1 = z_{\min}$ and $z_M = z_{\max}$. Denote the grid with the variable name, i.e. $z \equiv \{z_i\}_{i=1}^M$.

- Denote the distance between the grid points as the *backwards* difference

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

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

- Assume $\Delta_{1,-} = \Delta_{1,+}$ and $\Delta_{M,+} = \Delta_{M,-}$, due to ghost points, z_0 and z_{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

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

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

- Reflecting barrier conditions:

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

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

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 $L_1^- v(z)$ 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):

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

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, (5) implies

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

at the lower bound.

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

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

at the upper bound.

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

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

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

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

Similarly, by (6), we have

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

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

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

at the upper bound.

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

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

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

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

1.2 Irregular grids

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

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

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

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

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

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

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

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

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

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

Similarly, by (6), we have

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

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

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

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

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

at the upper bound.

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

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

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

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

1.3 Differential operators by basis

Define the following basis matrices:

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

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

$$
\tag{36}
$$

and the boundary conditions for the reflecting conditions:

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

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

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

$$L_1^- = \mathrm{diag}(\Delta_-)^{-1}U_1^- - B_1 \tag{42}$$
$$L_1^+ = \mathrm{diag}(\Delta_+)^{-1}U_1^+ + B_M \tag{43}$$
$$L_2 = \mathrm{diag}\left[\frac{1}{2}(\Delta_+ + \Delta_-)\Delta_+\right]^{-1}U_1^+ - \mathrm{diag}\left[\frac{1}{2}(\Delta_+ + \Delta_-)\Delta_-\right]^{-1}U_1^- + B_1 + B_M \tag{44}$$

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

$$L_2 = 2\left[\mathrm{diag}\left((\Delta_+ + \Delta_-)^{-1}\Delta_+^{-1}\right)U_1^+ - \mathrm{diag}\left((\Delta_+ + \Delta_-)^{-1}\Delta_-^{-1}\right)U_1^-\right] + B_1 + B_M \tag{45}$$
$$= 2\mathrm{diag}\left((\Delta_+ + \Delta_-)^{-1}\right)\left[\mathrm{diag}\left(\Delta_+^{-1}\right)U_1^+ - \mathrm{diag}\left(\Delta_-^{-1}\right)U_1^-\right] + B_1 + B_M \tag{46}$$

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

$$-2\left[(\Delta_+ + \Delta_-)^{-1}\Delta_+^{-1} + (\Delta_+ + \Delta_-)^{-1}\Delta_-^{-1}\right] = -2(\Delta_+ + \Delta_-)^{-1}(\Delta_+^{-1} + \Delta_-^{-1}) \tag{47}$$
$$= -2(\Delta_+ + \Delta_-)^{-1}(\Delta_+^{-1}\Delta_-^{-1})(\Delta_+ + \Delta_-) \tag{48}$$
$$= -2(\Delta_+^{-1}\Delta_-^{-1}) \tag{49}$$

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

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