Numerical Spectral Method

Let $\vec{u} = \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_{n-1} \end{bmatrix}$ be periodic

where u_j are measurements of true periodic function u on $[0, 2\pi]$

$$u_j = u\left(\frac{2\pi}{n} j\right), \quad j = 0, \dots, n-1$$

Given a matrix $\tilde{D}$,

e.g. $\tilde{D} = \frac{n}{4\pi} \begin{bmatrix} 0 & 1 & & \cdots & 1 \\ -1 & 0 & 1 & & \\ \vdots & & \ddots & & \vdots \\ & & & \ddots & \\ 1 & & \cdots & -1 & 0 \end{bmatrix}$

To show whether $\tilde{D}$ is a discretization of differential operator $\frac{d}{dx}$ or not,

consider $\tilde{D}\vec{u}$.

Write:

$$\tilde{D}\vec{u} = \begin{bmatrix} (\tilde{D}\vec{u})_0 \\ (\tilde{D}\vec{u})_1 \\ \vdots \\ (\tilde{D}\vec{u})_{n-1} \end{bmatrix}$$

$$(\tilde{D}\vec{u})_j = \frac{n}{4\pi}\left((\vec{u})_{j+1} - (\vec{u})_{j-1}\right)$$

$$= \frac{n}{4\pi}\left(u_{j+1} - u_{j-1}\right)$$

$$(1) - u(x+h) = u(x) + u'(x)h + \frac{u''(x)}{2}h^2 + \cdots$$

$$(2) - u(x-h) = u(x) - u'(x)h + \frac{u''(x)}{2}h^2 + \cdots$$

$(1) - (2)$:

$$u(x+h) - u(x-h) = u'(x)(2h) + \cdots$$

$$u'(x) \approx \frac{u(x+h) - u(x-h)}{2h}$$

If $h = \frac{2\pi}{n}$,

we have $$u'(x_j) \approx \frac{u(x_j+h) - u(x_j-h)}{2(2\pi/n)}$$

$$= \frac{n}{4\pi}\left(u_{j+1} - u_{j-1}\right)$$

$$= (\tilde{D}\vec{u})_j.$$

consider $u(x) = e^{ikx}$, $k \in \mathbb{N}$.

$$\frac{d}{dx} u(x) = ik\, e^{ikx} = ik\, u(x).$$

For simpler notation, write $h = \frac{2\pi}{n}$.

$$\overrightarrow{e^{ikx}} = \begin{bmatrix} e^{ikx_0} \\ e^{ikx_1} \\ \vdots \\ e^{ikx_{n-1}} \end{bmatrix} = \begin{bmatrix} e^{ik(0)h} \\ e^{ik(1)h} \\ \vdots \\ e^{ik(n-1)h} \end{bmatrix}$$

$$(\tilde{D}\, \overrightarrow{e^{ikx}})_j = \frac{n}{4\pi}\left(e^{ikx_{j+1}} - e^{ikx_{j-1}}\right)$$

$$= \frac{1}{2h}\left(e^{ik(j+1)h} - e^{ik(j-1)h}\right)$$

$$= \frac{1}{2h}\left(e^{ikh} - e^{-ikh}\right) \underline{e^{ikjh}} = e^{ikx_j}$$

$$= \frac{1}{2h}\left(\cos kh + i\sin kh - \cos kh + i \sin kh\right) e^{ikx_j}$$

$$= \frac{i}{h} \sin kh\, e^{ikx_j} = ik \frac{\sin kh}{kh} e^{ikx_j}$$

$$ik \frac{\sin kh}{kh} \to ik \text{ as } h \to 0.$$

$$\tilde{D}\,\overrightarrow{e^{ikx}} = \begin{bmatrix} (\tilde{D}\,\overrightarrow{e^{ikx}})_0 \\ \vdots \\ (\tilde{D}\,\overrightarrow{e^{ikx}})_{n-1} \end{bmatrix}$$

$\lambda_k = \frac{i}{h}\sin kh$,

$$= \begin{bmatrix} \lambda_k\, e^{ikx_0} \\ \vdots \\ \lambda_k\, e^{ikx_{n-1}} \end{bmatrix}$$

$$= \lambda_k \begin{bmatrix} e^{ikx_0} \\ \vdots \\ e^{ikx_{n-1}} \end{bmatrix}$$

$$= \lambda_k\, \overrightarrow{e^{ikx}}$$

$\therefore$ $\overrightarrow{e^{ikx}}$ is an eigenvector of $\tilde{D}$

with eigenvalue $= \frac{i}{h}\sin kh$

Higher degree differential operators:

$$\frac{d^2}{dx^2} = \underline{\frac{d}{dx}}\left(\underline{\frac{d}{dx}}\right)$$

You can use one method to discretize $\frac{d}{dx}$ and one method to discretize $\frac{d}{dx}$ (can be the same).

$$\frac{du}{dx} \approx \frac{u(x+h/2) - u(x-h/2)}{h}$$

$$\frac{d^2u}{dx^2} \approx \frac{u'(x+h/2) - u'(x-h/2)}{h}$$

$$\approx \frac{[u((x+h/2)+h/2) - u((x-h/2)+h/2)] - [u((x-h/2)+h/2) - u((x-h/2)-h/2)]}{h^2}$$

$$= \frac{u(x+h) - 2u(x) + u(x-h)}{h^2}$$

$$\therefore \tilde{\tilde{D}} = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & \cdots & & 1 \\ 1 & -2 & 1 & & \\ & & \ddots & \ddots & \\ 1 & & & 1 & -2 \end{bmatrix}$$

Example

$$\begin{cases} \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2}, & x \in (0, 2\pi),\ t > 0 \\ u(x, 0) = f(x) \\ u(0, t) = u(2\pi, t) \end{cases}$$

Discretize $[0, 2\pi]$ into n parts,

$$x_j = \frac{2\pi}{n} j$$

discretize t:

$$t_k = k \Delta t$$

$$j = 0, 1, \cdots, n-1, \quad k = 0, 1, \cdots$$

$$u_{j,k} = u(x_j, t_k)$$

PDE:

$$\frac{u_{j,k+1} - u_{j,k}}{\Delta t} = \frac{u_{j+1,k} - 2u_{j,k} + u_{j-1,k}}{h^2}$$

For each k, iDFT =>

$$\vec{u}_k = \begin{bmatrix} u_{0,k} \\ u_{1,k} \\ \vdots \\ u_{n-1,k} \end{bmatrix} = \sum_{m=0}^{n-1} \hat{u}_{k,m} \, \vec{e^{imx}}$$

Then:

$$\frac{1}{\Delta t}\left(\vec{u}_{k+1} - \vec{u}_k\right) = \tilde{\tilde{D}}\, \vec{u}_k$$

$$= \sum_{m=0}^{n-1} \hat{u}_{k,m} \left(\tilde{\tilde{D}}\, \overrightarrow{e^{imx}}\right)$$

$$= \sum_{m=0}^{n-1} \hat{u}_{k,m}\, \lambda_m\, \overrightarrow{e^{imx}}$$

$$\Rightarrow \quad \vec{u}_{k+1} = \vec{u}_k + \Delta t \left(\sum_{m=0}^{n-1} \hat{u}_{k,m}\, \lambda_m\, \overrightarrow{e^{imx}}\right)$$

$$\Rightarrow \quad \sum_{m=0}^{n-1} \hat{u}_{k+1,m}\, \overrightarrow{e^{imx}} = \sum_{m=0}^{n-1} \left(1 + \lambda_m \Delta t\right) \hat{u}_{k,m}\, \overrightarrow{e^{imx}}$$

Note Initial Condition:

$$u(x,0) = f(x)$$

$$\Rightarrow \quad \vec{u}_0 = \vec{f} \quad \Rightarrow \quad \hat{u}_{0,m} = \hat{f}_m$$

Hence, we can iteratively solve all $\hat{u}_{k,m}$, $k \geq 1$.

to recover $\vec{u}_k$

Exercise

Construct and verify a discretization for $\frac{d^3}{dx^3}$

Write down the matrix form.

Find the eigenvalues and eigenvectors of the matrix.

Solution

$$u'''(x) \approx \frac{u''(x+h) - u''(x)}{h}$$

$$\approx \frac{\dfrac{u'(x+2h) - u'(x+h)}{h} - \dfrac{u'(x+h) - u'(x)}{h}}{h}$$

$$= \frac{u'(x+2h) - 2u'(x+h) + u'(x)}{h^2}$$

$$\approx \frac{\left[\dfrac{u(x+3h) - u(x+2h)}{h} - 2\,\dfrac{u(x+2h) - u(x+h)}{h} + \dfrac{u(x+h) - u(x)}{h}\right]}{h^2}$$

$$= \frac{u(x+3h) - 3u(x+2h) + 3u(x+h) - u(x)}{h^3}$$

$$(1) - u(x+3h) = u(x) + u'(x)(3h) + u''(x)(3h)^2/2 + u'''(x)(3h)^3/6 + O(h^4)$$

$$(2) - u(x+2h) = u(x) + u'(x)(2h) + u''(x)(2h)^2/2 + u'''(x)(2h)^3/6 + O(h^4)$$

$$(3) - u(x+h) = u(x) + u'(x)(h) + u''(x)(h)^2/2 + u'''(x)(h)^3/6 + O(h^4)$$

$(1) - 3(2) + 3(3) - u(x)$:

$$LHS = u(x+3h) - 3u(x+2h) + 3u(x+h) - u(x)$$

$$RHS = \left.\begin{aligned} &(1-3+3-1)\, u(x) \\ &+ (1\times 3 - 3\times 2 + 3\times 1)\, h\, u'(x) \\ &+ (1\times 3^2 - 3\times 2^2 + 3\times 1^2)\, \frac{h^2}{2} u''(x) \end{aligned}\right\} = 0$$

$$+ \underbrace{(1\times 3^3 - 3\times 2^3 + 3\times 1^3)}_{(27-24+3)/6 = 1} \frac{h^3}{6} u'''(x) + O(h^4)$$

$$= h^3 u'''(x) + O(h^4)$$

$$\tilde{D} = \begin{bmatrix} -1 & 3 & -3 & 1 & \cdots & 0 \\ 0 & -1 & 3 & -3 & 1 & \\ \vdots & & \ddots & & & \vdots \\ 3 & -3 & 1 & \cdots & & -1 \end{bmatrix}$$

$$\left(\tilde{D} \vec{e^{ikx}} \right)_j = \frac{e^{ikx_{j+3}} - 3e^{ikx_{j+2}} + 3e^{ikx_{j+1}} - e^{ikx_j}}{h^3}$$

$$= \underbrace{\left(\frac{e^{ik3h} - 3e^{ik2h} + 3e^{ikh} - 1}{h^3} \right)}_{\text{Can be further simplify}} e^{ikx_j}$$

In fact, in this case,

$$\tilde{D} = \left(\frac{1}{h} \begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ 1 & & & -1 \end{bmatrix} \right)^3 = D^3$$

is a cube of discretization of $\frac{d}{dx}$.

the eigenvalue of $\tilde{D}$ is cube of those of D.