Lecture 10:

Numerical Spectral method

Since $\{\overrightarrow{e^{ikx}}\}_{k=0}^{N-1}$ is a basis. We can write:

$$\vec{u} = \sum_{k=0}^{N-1} \hat{u}_k \overrightarrow{e^{ikx}} \quad \text{and} \quad \vec{f} = \sum_{k=0}^{N-1} \hat{f}_k \overrightarrow{e^{ikx}}$$

$\mathbb{C}$

In other words, for each j, $f_j = f(x_j) = \sum_{k=0}^{N-1} \hat{f}_k \left(\overrightarrow{e^{ikx}}\right)_j$

$$= \sum_{k=0}^{N-1} \hat{f}_k e^{ikx_j}$$

(DFT!)

$\therefore$ $\hat{f}_k$ can be determined by DFT.

To solve $\frac{d^2u}{dx^2} = f$, we approximate it by

$$\tilde{D}\vec{u} = \vec{f}.$$

Now, $\tilde{D}\vec{u} = \vec{f}$ becomes:

$$\tilde{D}\left(\sum_{k=0}^{N-1} \hat{u}_k \overrightarrow{e^{ikx}}\right) = \sum_{k=0}^{N-1} \hat{f}_k \overrightarrow{e^{ikx}}$$

$$\Longleftrightarrow \quad \sum_{k=0}^{N-1} \hat{u}_k \underset{\overset{\parallel}{(-\lambda k^2)\overrightarrow{e^{ikx}}}}{\tilde{D}\,\overrightarrow{e^{ikx}}} = \sum_{k=0}^{N-1} \hat{f}_k \overrightarrow{e^{ikx}}$$

$$\Longleftrightarrow \quad \sum_{k=0}^{N-1} \hat{u}_k (-\lambda k^2) \overrightarrow{e^{ikx}} = \sum_{k=0}^{N-1} \hat{f}_k \overrightarrow{e^{ikx}}$$

Comparing coefficients, we get

$$\underbrace{-\lambda k^2}_{\text{known}}\ \underbrace{\hat{u}_k}_{\text{unknown}} = \underbrace{\hat{f}_k}_{\text{known}} \quad \text{for } k = 0, 1, 2, \ldots, N-1$$

(algebraic equation)

For $k = 1, 2, \ldots, N-1$, we have: $\hat{u}_k = \hat{f}_k / (-\lambda_k^2)$.

For $k=0$, $\lambda_k = 0$!!

We consider a special solution such that:

$$\hat{u}_0 = \frac{u_0 + u_1 + \ldots + u_{N-1}}{N} = 0 \qquad \text{(Zero - mean solution)}$$

Then, we can set $\hat{u}_0 = 0$

Note that $\hat{f}_0 = -\lambda_0^2 \hat{u}_0 = 0 \Rightarrow \dfrac{f_0 + f_1 + \ldots + f_{N-1}}{N} = 0$

This is consistent with the compatible condition of f:

$$\underbrace{\int_0^{2\pi} f(x)\,dx}_{\hat{f}_0} = \int_0^{2\pi} u''(x)\,dx = u'(x)\Big|_0^{2\pi} = 0 \quad (\text{Periodic})$$

Once $\hat{u}_k$ is obtained for $k = 0, 1, 2, \dots, N-1$, $\vec{u}$ can be obtained by:

$$\vec{u} = \begin{pmatrix} u(x_0) \\ u(x_1) \\ \vdots \\ u(x_{N-1}) \end{pmatrix} = \sum_{k=0}^{N-1} \hat{u}_k \overrightarrow{e^{ikx}}$$

(inverse DFT)

or $\vec{u} = A_\omega \begin{pmatrix} \hat{u}_0 \\ \hat{u}_1 \\ \vdots \\ \hat{u}_{N-1} \end{pmatrix}$ where $A_\omega = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & \omega & & \omega^{N-1} \\ \vdots & \omega^2 & & \vdots \\ \vdots & \vdots & & \vdots \\ 1 & \omega^{N-1} & & \omega^{(N-1)^2} \end{pmatrix}$

$\omega = e^{i\frac{2\pi}{N}}$

(Matrix multiplication)

<u>Remark</u>: For any other solution $\vec{u}_*$, $\vec{u}_* = \vec{u} + c\begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$ for some constant c.

c is determined by other condition (such as boundary condition)

Example: Consider: $a\frac{d^2u}{dx^2} + b\frac{du}{dx} = f$ for $x \in [0, 2\pi]$.

This time, we approximate $\frac{d^2u}{dx^2}$ by:

$$(*) \quad \frac{d^2u}{dx^2}(x_j) \approx \frac{u_{j-2} - 2u_j + u_{j+2}}{4h^2} \quad \text{for } j = 0, 1, 2, \dots, N-1$$

Again, we assume $u_{-1} = u_{N-1}$, $u_1 = u_{N+1}$, $u_{-2} = u_{N-2}$, ..., etc

Motivation: ① $u(x_j + 2h) \approx u(x_j) + 2h\,u'(x_j) + 2h^2 u''(x_j)$

② $u(x_j - 2h) \approx u(x_j) - 2h\,u'(x_j) + 2h^2 u''(x_j)$

① + ②: $u(x_{j+2}) + u(x_{j-2}) - 2u(x_j) = 4h^2 u''(x_j)$

This time, we approximate $\frac{du}{dx}$ as:

$$(**) \quad \frac{du}{dx}(x_j) \approx \frac{u_{j+1} - u_{j-1}}{2h}$$

Denote (**) in matrix form as:

$$\begin{pmatrix} u'(x_0) \\ u'(x_1) \\ \vdots \\ u'(x_{N-1}) \end{pmatrix} = \tilde{D}\vec{u} \quad \text{where} \quad \tilde{D} = \frac{1}{2h}\begin{pmatrix} 0 & 1 & & & -1 \\ -1 & 0 & \ddots & 0 & \\ & \ddots & \ddots & \ddots & \\ & 0 & \ddots & \ddots & 1 \\ 1 & & & -1 & 0 \end{pmatrix}$$

Denote (*) in matrix form as:

$$\begin{pmatrix} u''(x_0) \\ u''(x_1) \\ \vdots \\ u''(x_{N-1}) \end{pmatrix} = D\vec{u} \quad \text{where} \quad D = \frac{1}{4h^2}\begin{pmatrix} -2 & 0 & 1 & & \cdots & 1 & 0 \\ 0 & -2 & 0 & 1 & & & 0 \\ 1 & 0 & \ddots & 0 & \ddots & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \ddots & 1 \\ & 0 & & \ddots & \ddots & \ddots & 0 \\ 0 & 1 & & & 1 & 0 & -2 \end{pmatrix}$$

Remark: $D = \tilde{D}^2$.

Claim: $e^{i\overrightarrow{kx}}$ is an eigenvector of $\tilde{D}$ and D.

Proof:

$$\left(D e^{i\overrightarrow{kx}}\right)_j = \frac{e^{ikx_{j-2}} - 2e^{ikx_j} + e^{ikx_{j+2}}}{4h^2}$$

$$= \frac{e^{ikx_j}\left(e^{-2ikh} - 2 + e^{2ikh}\right)}{4h^2}$$

$$= \underbrace{\left(-\frac{\sin^2(kh)}{h^2}\right)}_{\tilde{\lambda}_k^2} e^{ikx_j}$$

$$\therefore D e^{i\overrightarrow{kx}} = \tilde{\lambda}_k^2 e^{i\overrightarrow{kx}}.$$

Also, $\tilde{D} e^{i\overrightarrow{kx}} = \dfrac{e^{ikx_{j+1}} - e^{ikx_{j-1}}}{2h} = e^{ikx_j}\dfrac{\left(e^{ikh} - e^{-ikh}\right)}{2h}$

$$= \underbrace{\left(\frac{i\sin(kh)}{h}\right)}_{\tilde{\lambda}_k} e^{ikx_j}$$

$$\therefore \tilde{D} e^{i\overrightarrow{kx}} = \tilde{\lambda}_k e^{i\overrightarrow{kx}}$$

Now, $a\dfrac{d^2u}{dx^2} + b\dfrac{du}{dx} = f$ can be discretized as:

$$a\tilde{D}^2\vec{u} + b\tilde{D}\vec{u} = \vec{f}$$ subject to the periodic condition.

Recall: $\{\overrightarrow{e^{ikx}}\}_{k=0}^{N-1}$ is a basis for $\mathbb{C}^N$

Again, let $\vec{u} = \sum_{k=0}^{N-1} \hat{u}_k \overrightarrow{e^{ikx}}$ and $\vec{f} = \sum_{k=0}^{N-1} \hat{f}_k \overrightarrow{e^{ikx}}$

Then: $a\tilde{D}^2\left(\sum_{k=0}^{N-1} \hat{u}_k \overrightarrow{e^{ikx}}\right) + b\tilde{D}\left(\sum_{k=0}^{N-1} \hat{u}_k \overrightarrow{e^{ikx}}\right) = \sum_{k=0}^{N-1} \hat{f}_k \overrightarrow{e^{ikx}}$

$$\Longleftrightarrow \sum_{k=0}^{N-1} \left(a\tilde{\lambda}_k^2 + b\tilde{\lambda}_k\right) \hat{u}_k \overrightarrow{e^{ikx}} = \sum_{k=0}^{N-1} \hat{f}_k \overrightarrow{e^{ikx}}$$

Comparing coefficients, we get: $\left(a\tilde{\lambda}_k^2 + b\tilde{\lambda}_k\right)\hat{u}_k = \hat{f}_k$ for $k = 0, \ldots, N-1$

(algebraic equation)

For $k=0$ and $\frac{N}{2}$, $\tilde{\lambda}_k = 0$. We set $\hat{u}_0 = 0 = \hat{u}_{\frac{N}{2}}$.

In general, we set:

$$\hat{u}_k = \begin{cases} \hat{f}_k / (a\tilde{\lambda}_k^2 + b\tilde{\lambda}_k) & \text{for } k \neq 0, N/2 \\ 0 & \text{for } k=0 \text{ or } k = N/2 \end{cases}$$

$\vec{u}$ can be obtained by inverse DFT:

$$\begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_{N-1} \end{pmatrix} = A_\omega \begin{pmatrix} \hat{u}_0 \\ \hat{u}_1 \\ \vdots \\ \hat{u}_{N-1} \end{pmatrix}$$

<u>Question:</u> How about the general solution?

<u>Answer:</u> Examine $N(a\tilde{D}^2 + b\tilde{D})$, the null space.

Claim: $N(a\tilde{D}^2 + b\tilde{D}) = \operatorname{span}\{\overrightarrow{e^{i(0)x}}, \overrightarrow{e^{i(\frac{N}{2})x}}\}$

$$= \operatorname{span}\left\{ \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}, \begin{pmatrix} e^{i(\frac{N}{2})x_1} \\ \vdots \\ e^{i(\frac{N}{2})x_{N-1}} \end{pmatrix} \right\}$$

Proof: $a\tilde{D}^2 + b\tilde{D}$ has two eigenvectors whose eigenvalue is 0.

These eigenvectors are $\overrightarrow{e^{i(0)x}}$ and $\overrightarrow{e^{i(\frac{N}{2})x}}$.

$$N(a\tilde{D}^2 + b\tilde{D}) = \text{eigenspace of eigenvalue} = 0$$

$$= \operatorname{span}\{\overrightarrow{e^{i(0)x}}, \overrightarrow{e^{i(\frac{N}{2})x}}\}.$$

Thus, general sol: $\vec{u}^* = \vec{u} + c_1 \overrightarrow{e^{i(0)x}} + c_2 \overrightarrow{e^{i(\frac{N}{2})x}}$

for some c_1 and c_2.

c_1 and c_2 can be determined by certain conditions (such as boundary conditions)

Main idea of numerical spectral method

Diff. eqt $\longrightarrow$ Algebraic eqt $\longrightarrow$ solution $\vec{u}$

(e.g. $\frac{d^2u}{dx^2} = f$)

DFT on $\vec{f}$ $\left(\frac{\overline{A_w}}{n}\vec{f}\right)$ Fast?

Fast!

inverse DFT on $\hat{u}$ $\left(A_w \hat{u}\right)$ Fast?

Remark: • To develop an efficient numerical spectral method, we need to compute $A_w \hat{u}$ and $\frac{\overline{A_w}}{n}\vec{f}$ fast.

• Computational cost for $\underset{(n \times n)}{A_w} \hat{u}$ is $O(n^2)$.

Goal: Reduce the computational cost to $O(n \log n)$

e.g. $n = 2^{10}$, $n^2 = 2^{20}$, $n \log n = 10 \cdot 2^{10} < 2^{14}$. $\therefore$ $2^6 = 64$ times faster!