Lecture 12:

Main idea of numerical spectral method

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

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

DFT on $\vec{f}$ $\left(\dfrac{\overline{A_w}}{n}\vec{f}\right)$

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 $\dfrac{\overline{A_w}}{n}\vec{f}$ 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!

Fast Fourier Transform (FFT) (Colley and Tukey, 1965)

Let $F_n = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & \omega_n & \cdots & \omega_n^{n-1} \\ \vdots & \vdots & & \\ 1 & \omega_n^{n-1} & \cdots & \omega_n^{(n-1)^2} \end{pmatrix}$ where $\omega_n = e^{i\left(\frac{2\pi}{n}\right)}$.

Let $\vec{y} = F_n \vec{x}$, where $\vec{y} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{n-1} \end{pmatrix}$ and $\vec{x} = \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{pmatrix}$. Suppose $n = 2m$.

Then, for each $0 \le j \le n-1$,

$$y_j = \sum_{k=0}^{n-1} \omega_n^{jk} x_k = \sum_{k=0}^{2m-1} \omega_{2m}^{kj} x_k .$$

Divide $k = 0, 1, 2, \ldots, 2m-1$ into two parts:

<u>Part 1:</u> $0, 2, 4, 6, \ldots, 2(m-1)$ (Even)

<u>Part 2:</u> $1, 3, 5, 7, \ldots, 2m-1$ (Odd)

Then: $$y_j = \underbrace{\sum_{k=0}^{m-1} \omega_n^{2kj} x_{2k}}_{\text{Part 1}} + \underbrace{\sum_{k=0}^{m-1} \omega_n^{(2k+1)j} x_{2k+1}}_{\text{Part 2}}$$

$$= \sum_{k=0}^{m-1} \omega_m^{kj} \overset{(\vec{x}')_k}{x_{2k}} + \sum_{k=0}^{m-1} \omega_n^{j} \omega_m^{kj} \overset{(\vec{x}'')_k}{x_{2k+1}} \qquad \left(\because \ \omega_{2m}^{2k} = e^{i\left(\frac{2\pi}{2m}\right)2k} = e^{i\left(\frac{2\pi}{m}\right)k} = \omega_m^k \right)$$

Denote $\vec{x}' = \begin{pmatrix} x_0 \\ x_2 \\ \vdots \\ x_{2m-2} \end{pmatrix}$, $\vec{x}'' = \begin{pmatrix} x_1 \\ x_3 \\ \vdots \\ x_{2m-1} \end{pmatrix}$. Let $\vec{y}' = F_m \vec{x}'$ and $\vec{y}'' = F_m \vec{x}''$.

$$\therefore \ y_j = (\overset{m\times m}{F_m} \vec{x}')_j + \omega_n^j (\overset{m\times m}{F_m} \vec{x}'')_j \quad \text{for } j = 0, 1, 2, \dots, m-1$$

$$= \underbrace{(\vec{y}')_j}_{\text{j-th entry of } \vec{y}'} + \omega_n^j \underbrace{(\vec{y}'')_j}_{\text{j-th entry of } \vec{y}''}$$

$$y_{j+m} = \sum_{k=0}^{m-1} \omega_n^{2k(j+m)} x_{2k} + \sum_{k=0}^{m-1} \omega_n^{(2k+1)(j+m)} x_{2k+1} \quad \text{for } j = 0, 1, 2, \dots, m-1$$

Capture $y_m, y_{m+1}, \dots, y_{2m-1}$

$$= \sum_{k=0}^{m-1} \omega_m^{kj}\, \omega_m^{km} (\vec{x}\,')_k + \sum_{k=0}^{m-1} \omega_m^{k(j+m)}\, \omega_n^{j+m} (\vec{x}\,'')_k$$

$$\omega_m^{km} = e^{i\left(\frac{2\pi}{m}\right)km} = 1$$

$$\omega_m^{k(j+m)} = \omega_m^{kj}\,\omega_m^{km} = \omega_m^{kj}$$

$$\omega_n^{j+m} = \omega_n^{j}\,\omega_n^{m} = \omega_n^{j}\, e^{i\left(\frac{2\pi}{2m}\right)\cdot m} = -\omega_n^{j}$$

$$\therefore\ y_{j+m} = \sum_{k=0}^{m-1} \omega_m^{kj} (\vec{x}\,')_k - \omega_n^{j} \sum_{k=0}^{m-1} \omega_m^{kj} (\vec{x}\,'')_k$$

$$y_{j+m} = (\underbrace{F_m}_{m\times m} \vec{x}\,')_j - \omega_n^{j} (\underbrace{F_m}_{m\times m} \vec{x}\,'')_j \quad \text{for } j = 0, 1, 2, \dots, m-1$$

Note: $n \times n$ matrix multiplication becomes $\frac{n}{2} \times \frac{n}{2} = m \times m$ matrix multiplication.

For simplicity, we denote:

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \otimes \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} v_1 w_1 \\ v_2 w_2 \\ \vdots \\ v_n w_n \end{pmatrix}$$

Then:

$$\begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{m-1} \end{pmatrix} = \vec{y}\,' + \begin{pmatrix} \omega_n^0 \\ \omega_n^1 \\ \vdots \\ \omega_n^{m-1} \end{pmatrix} \otimes \vec{y}\,'' \quad \text{and} \quad \begin{pmatrix} y_m \\ y_{m+1} \\ \vdots \\ y_{2m-1} \end{pmatrix} = \vec{y}\,' - \begin{pmatrix} \omega_n^0 \\ \omega_n^1 \\ \vdots \\ \omega_n^{m-1} \end{pmatrix} \otimes \vec{y}\,''$$

Summary of FFT

Step 1: Split $\vec{x}$ into $\vec{x}\,' = \begin{pmatrix} x_0 \\ x_2 \\ \vdots \\ x_{2(m-1)} \end{pmatrix}$ and $\vec{x}\,'' = \begin{pmatrix} x_1 \\ x_3 \\ \vdots \\ x_{2m-1} \end{pmatrix}$

Step 2: Compute $\underset{O(m^2)}{\vec{y}\,' = F_m \vec{x}\,'}$ and $\underset{O(m^2)}{\vec{y}\,'' = F_m \vec{x}\,''}$, where $F_m = \overset{m \times m}{\overset{\shortparallel}{\frac{n}{2} \times \frac{n}{2}}}$ matrix

Step 3: Compute:

$$\begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{m-1} \end{pmatrix} = \vec{y}\,' + \overbrace{\begin{pmatrix} \omega_n^0 \\ \omega_n^1 \\ \vdots \\ \omega_n^{m-1} \end{pmatrix}}^{\vec{\omega}_m} \otimes \vec{y}\,'' \quad O(m) \quad \text{and} \quad \begin{pmatrix} y_m \\ y_{m+1} \\ \vdots \\ y_{2m-1} \end{pmatrix} = \vec{y}\,' - \overbrace{\begin{pmatrix} \omega_n^0 \\ \omega_n^1 \\ \vdots \\ \omega_n^{m-1} \end{pmatrix}}^{\vec{\omega}_m} \otimes \vec{y}\,'' \quad O(m)$$

Remark: Computational cost : $\mathcal{O}(m^2) + \mathcal{O}(m)$ (multiplication + addition)

$\approx$

$\mathcal{O}(m^2)$

Computational cost for FFT: Assume $n = 2^l$.

Let C_m = computational cost of F_m. Then $C_1 = 1$.

Claim: $C_{2m} = 2C_m + 3m$

Proof: **Step 2:** $\vec{y}' = F_m \vec{x}'$, $\vec{y}'' = F_m \vec{x}''$ $(= 2C_m)$

Step 3: $y_j = \vec{y}_j' + \omega_n^j \vec{y}_j''$

$y_{j+m} = \vec{y}_j' - \omega_n^j \vec{y}_j''$

for $j = 0, 1, 2, \dots, m-1$

(= 1 multiplication + 1 addition + 1 substraction)

$\Downarrow$

Total : $3m$

$\therefore$ $C_{2m} = 2C_m + 3m$.

Now, $n = 2^{\ell}$.

$$\therefore \quad C_{2^{\ell}} = 2C_{2^{\ell-1}} + 3 \cdot 2^{\ell-1}.$$

$$\therefore \quad 2^{-\ell}C_{2^{\ell}} = 2^{-(\ell-1)}C_{2^{\ell-1}} + \frac{3}{2} = 2^{-(\ell-2)}C_{2^{\ell-2}} + 2\left(\frac{3}{2}\right)$$

$$= \vdots$$

$$= 2^{0}C_{2^{0}} + \ell\left(\frac{3}{2}\right) = 1 + \frac{3}{2}\ell$$

$$\therefore \quad C_{2^{\ell}} = \underbrace{2^{\ell}}_{n} + \frac{3}{2}\overbrace{\ell}^{\log_2 n}\underbrace{2^{\ell}}_{n} = n + \frac{3}{2}n\log_2 n = O(n\log_2 n)$$

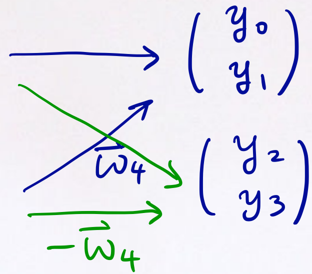
Butterfly diagram (Algorithmic visualization)

Consider F_4 $(4 \times 4$ matrix$)$.

[Recall: $\vec{y}_e = \vec{y}\,' = F_m \vec{x}\,'$
$\vec{y}_o = \vec{y}\,'' = F_m \vec{x}\,''$.
Denote $\vec{x}\,' := \vec{x}_e$, $\vec{x}\,'' = \vec{x}_o$]

$$\vec{y}_e := F_2 \vec{x}_e = \begin{pmatrix} \cdot \\ \cdot \end{pmatrix}, \qquad \vec{x}_e = \begin{pmatrix} x_0 \\ x_2 \end{pmatrix}$$

$$\vec{y}_o := F_2 \vec{x}_o = \begin{pmatrix} \cdot \\ \cdot \end{pmatrix}, \qquad \vec{x}_o = \begin{pmatrix} x_1 \\ x_3 \end{pmatrix}$$



$$\vec{\omega}_4 = \begin{pmatrix} \omega_4^0 \\ \omega_4^1 \end{pmatrix}$$

Diagram means:

$$\begin{pmatrix} y_0 \\ y_1 \end{pmatrix} = \vec{y}_e + \vec{\omega}_4 \otimes \vec{y}_o$$

$$\begin{pmatrix} y_2 \\ y_3 \end{pmatrix} = \vec{y}_o - \vec{\omega}_4 \otimes \vec{y}_o$$

Depend on $\vec{y}_o$ and $\vec{y}_e$.

For $F_2\vec{x}_e$:

$$1 = F_1\vec{x}_{ee} = (x_0)$$
$$1 = F_1\vec{x}_{eo} = (x_2)$$

$\vec{\omega}_2^0$, $-\vec{\omega}_2^0$

$$\begin{pmatrix}\cdot\\ \cdot\end{pmatrix} = F_2\vec{x}_e = \vec{y}_e$$

For $F_2\vec{x}_o$:

$$1 = F_1\vec{x}_{oe} = (x_1)$$
$$1 = F_1\vec{x}_{oo} = (x_3)$$

$\vec{\omega}_2^0$, $-\vec{\omega}_2^0$

$$\begin{pmatrix}\cdot\\ \cdot\end{pmatrix} = F_2\vec{x}_o = \vec{y}_o$$

Remark:

$$\vec{x}_e = \begin{pmatrix}x_0\\ x_2\end{pmatrix}, \quad \vec{x}_o = \begin{pmatrix}x_1\\ x_3\end{pmatrix}$$

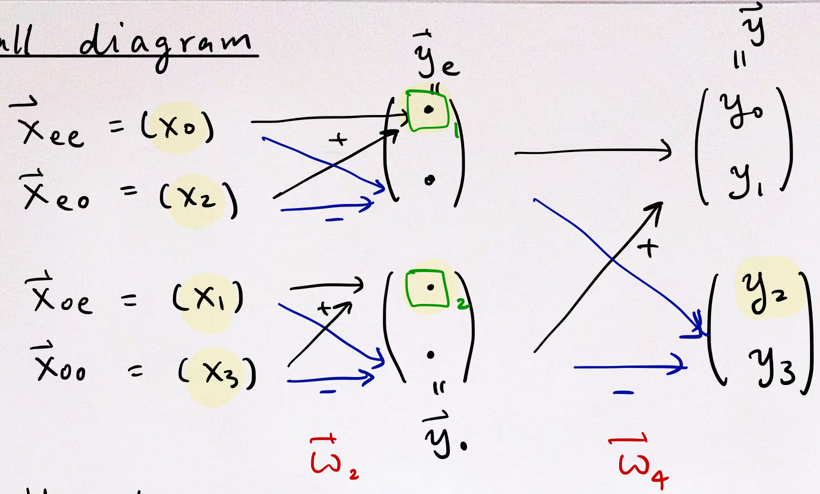
$$\vec{x}_{ee} = (x_0) \qquad \vec{x}_{oe} = (x_1)$$
$$\vec{x}_{eo} = (x_2) \qquad \vec{x}_{oo} = (x_3)$$

$$\vec{y}_e = \begin{pmatrix} x_0 + \vec{\omega}_2^0 \otimes (x_2) \\ x_0 - \vec{\omega}_2^0 \otimes (x_2)\end{pmatrix} = \begin{pmatrix} x_0 + x_2 \\ x_0 - x_2\end{pmatrix}$$

$$\vec{y}_o = \begin{pmatrix} x_1 + \vec{\omega}_2^0 \otimes (x_3) \\ x_1 - \vec{\omega}_2^0 \otimes (x_3)\end{pmatrix} = \begin{pmatrix} x_1 + x_3 \\ x_1 - x_3\end{pmatrix}$$

$$\vec{\omega}_2^0 = (\omega_2^0) = (1)$$

Overall diagram



(Butterfly diagram)

Using the diagram, find y_2.

$y_2 = \square_1 - (\vec{\omega}_4)_0 \square_2$; $\square_1 = x_0 + x_2$

$\quad = \square_1 - \square_2$; $\square_2 = x_1 + x_3$

$\therefore \; y_2 = x_0 + x_2 - (x_1 + x_3)$

Iterative method to solve huge linear system

Recall: Numerical spectral method handles periodic functions.

Consider: $(*)\quad \dfrac{d^2u}{dx^2} = f$, $u(0) = A$, $u(1) = B$

$x \in [0,1]$.

Partition $[0,1]$ into $x_j = jh$ where $h = \dfrac{1}{n+1}$

Then: $(*)$ is discretized as:

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = f(x_i)$$

for all $i = 1, 2, \ldots, n$

$$u_i \overset{\text{def}}{=} u(x_i)$$

or

$$\tilde{A}\begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} = \begin{pmatrix} f(x_1) - \frac{A}{h^2} \\ f(x_2) \\ \vdots \\ f(x_n) - \frac{B}{h^2} \end{pmatrix}$$

where

$$\tilde{A} = \frac{1}{h^2}\begin{pmatrix} -2 & 1 & & 0 \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ 0 & & 1 & -2 \end{pmatrix}$$

$$D = \begin{pmatrix} -2 & 1 & 0 & 1 \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ 1 & 0 & 1 & -2 \end{pmatrix}$$ has eigenvector $\overrightarrow{e^{ikx}}$

Question: How to solve BIG linear system?

Method 1: Gaussian elimination

Comp. cost : $O(n^3)$

Sol : exact.

Method 2: LU factorization.

Decompose $A = \underset{\text{lower}}{L}\,\underset{\text{upper}}{U}$

(If A is SPD, then $A = LL^T$ by Cholesky decomposition)

$LU\vec{x} = \vec{b}$ by solving $\left\{\begin{array}{l} L\vec{y} = \vec{b} \\ U\vec{x} = \vec{y} \end{array}\right.$ easy

Comp. cost : $O(n^3)$

Sol : exact.

Goal: Develop iterative method: find a sequence $\vec{x}_0, \vec{x}_1, \vec{x}_2, \ldots$ such that $\vec{x}_k \to \vec{x}^* =$ sol. of $A\vec{x} = \vec{f}$ as $k \to \infty$.

Remark: We can stop when error is small enough.

Method: Splitting method

Consider a linear system $A\vec{x} = \vec{f}$ where $A \in M_{n\times n}$ (n is BIG)

Split A as follows: $A = N + (A - N) = N - \underbrace{(N - A)}_{P}$

$= N - P$

Then: $A\vec{x} = \vec{f} \Leftrightarrow (N - P)\vec{x} = \vec{f} \Leftrightarrow N\vec{x} = P\vec{x} + \vec{f}$

Develop an iterative scheme as follows:

$$(*) \quad N\vec{x}^{n+1} = P\vec{x}^{n} + \vec{f}$$

If $\{\vec{x}^n\}_{n=1}^{\infty}$ converges, then it converges to the sol $\vec{x}^*$ of $A\vec{x} = \vec{f}$

<u>Remark:</u>

- N should be simple : easy to find inverse.
- N should have an inverse
- N should be "related to" A.