Lecture 17: FFT and structured matrices



School of Mathematical Sciences, Xiamen University

1. Discrete Fourier transform and its inverse

Definition 1

The discrete Fourier transform (DFT) is a mapping on \mathbb{C}^n given by

$$[\mathcal{F}_n{\{\mathbf{f}\}}]_i = \sum_{j=0}^{n-1} f_j \omega_n^{ij}, \quad i = 0, 1, \dots, n-1,$$

where $\omega_n = e^{-i2\pi/n}$ and $i = \sqrt{-1}$. The inverse DFT is given by

$$\left[\mathcal{F}_{n}^{-1}\{\mathbf{g}\}\right]_{i} = \frac{1}{n} \sum_{i=0}^{n-1} g_{j} \omega_{n}^{-ij}, \quad i = 0, 1, \dots, n-1.$$

• DFT and inverse DFT as matrix-vector products:

$$\mathcal{F}_n\{\mathbf{f}\} = \mathbf{F}_n\mathbf{f}, \quad \mathcal{F}_n^{-1}\{\mathbf{g}\} = \frac{1}{n}\mathbf{F}_n^*\mathbf{g} = \frac{1}{n}\overline{\mathbf{F}_n\overline{\mathbf{g}}}, \quad \mathbf{F}_n = \left[\omega_n^{ij}\right]_{i,j=0}^{n-1}.$$

• Discrete sine/cosine transform: DST, DCT, ...

2. The FFT algorithm

• For simplicity, we assume that $n=2^k$ and set m=n/2. Obviously,

$$\omega_m = \omega_n^2 = e^{-i2\pi/m}, \qquad \omega_m^m = 1, \qquad \omega_n^m = -1.$$

• Given any $\mathbf{f} = \begin{bmatrix} f_0 & f_1 & \cdots & f_{n-1} \end{bmatrix}^{\top} \in \mathbb{C}^n$, for $i = 0, 1, \dots, m-1$,

$$[\mathcal{F}_{n}\{\mathbf{f}\}]_{i} = \sum_{l=0}^{m-1} \omega_{n}^{i2l} f_{2l} + \sum_{l=0}^{m-1} \omega_{n}^{i(2l+1)} f_{2l+1}$$

$$= \sum_{l=0}^{m-1} \omega_{m}^{il} f_{2l} + \omega_{n}^{i} \sum_{l=0}^{m-1} \omega_{m}^{il} f_{2l+1}$$

$$= [\mathcal{F}_{m}\{\mathbf{f}_{e}\}]_{i} + \omega_{n}^{i} [\mathcal{F}_{m}\{\mathbf{f}_{o}\}]_{i},$$

where

$$\mathbf{f}_{e} = \begin{bmatrix} f_0 & f_2 & \cdots & f_{n-2} \end{bmatrix}^{\top}, \quad \mathbf{f}_{o} = \begin{bmatrix} f_1 & f_3 & \cdots & f_{n-1} \end{bmatrix}^{\top}.$$

• For $i = 0, 1, \ldots, m - 1$, we also have

$$[\mathcal{F}_{n}\{\mathbf{f}\}]_{m+i} = \sum_{l=0}^{m-1} \omega_{n}^{(m+i)2l} f_{2l} + \sum_{l=0}^{m-1} \omega_{n}^{(m+i)(2l+1)} f_{2l+1}$$

$$= \sum_{l=0}^{m-1} \omega_{m}^{il} f_{2l} - \omega_{n}^{i} \sum_{l=0}^{m-1} \omega_{m}^{il} f_{2l+1}$$

$$= [\mathcal{F}_{m}\{\mathbf{f}_{e}\}]_{i} - \omega_{n}^{i} [\mathcal{F}_{m}\{\mathbf{f}_{o}\}]_{i}.$$

• Let FFT(n) denote the number of flops required to evaluate $\mathbf{F}_n\mathbf{f}$ by a recursive algorithm. Given the vectors $\mathbf{F}_m\mathbf{f}_e$ and $\mathbf{F}_m\mathbf{f}_o$, only m multiplications, m additions and m subtractions are needed to evaluate $\mathcal{F}_n\{\mathbf{f}\}$. Hence,

$$FFT(n) = 3m + 2FFT(m) = 3n/2 + 2FFT(n/2)$$
.

Since FFT(1) = 0, then

$$FFT(n) = 3n/2 \times k = \frac{3}{2}n \log n.$$

3. Flop counts for frequently used algorithms

Matrix $(m \ge n)$	Operation or Factorization	Flops
	$\mathbf{b} = \mathbf{A}\mathbf{x}$	$2n^2$
$\mathbf{F} \in \mathbb{C}^{n \times n}$	$\mathbf{b} = \mathbf{F}\mathbf{x}$	$3n \log n/2$
$\mathbf{A}, \mathbf{B} \in \mathbb{C}^{n \times n}$	C = AB	$2n^3$
	\mathbf{A}^{-1}	$2n^3$
$\mathbf{A} \in \mathbb{C}^{n \times n}$	PA = LU	$2n^{3}/3$
$\mathbf{H} \in \mathbb{C}^{n \times n}$	$\mathbf{H} = \mathbf{L}\mathbf{U}$	$2n^2$
$\mathbf{T} \in \mathbb{C}^{n \times n}$	$\mathbf{T} = \mathbf{L}\mathbf{U}$	3n
	$\mathbf{A} = \mathbf{R}^* \mathbf{R}$	$n^{3}/3$
	$\mathbf{L}\mathbf{x} = \mathbf{b}$	n^2
	\mathbf{L}^{-1}	$2n^{3}/3$
$\mathbf{A} \in \mathbb{C}^{m \times n}$	$\mathbf{A}^*\mathbf{A} = \mathbf{R}^*\mathbf{R}$	$mn^2 + n^3/3$
	$\mathbf{Q}^*\mathbf{A}=\mathbf{R}$	$2(mn^2 - n^3/3)$
	$\mathbf{A} = \mathbf{Q}_n \mathbf{R}_n$	$2mn^2$
	$\mathbf{B} = \mathbf{U}^* \mathbf{A} \mathbf{V}$	$4(mn^2 - n^3/3)$
	$\mathbf{H} = \mathbf{Q}^* \mathbf{A} \mathbf{Q}$	$10n^{3}/3$
$\mathbf{A} \in \mathbb{C}^{n \times n}$	$T = Q^*AQ$	$4n^{3}/3$
$\mathbf{A} \in \mathbb{C}^{m \times n}$	$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^*$	$2mn^2 + 11n^3$
	$\mathbf{A} \in \mathbb{C}^{n \times n}$ $\mathbf{F} \in \mathbb{C}^{n \times n}$ $\mathbf{A}, \mathbf{B} \in \mathbb{C}^{n \times n}$ $\mathbf{A} \in \mathbb{C}^{n \times n}$ $\mathbf{A} \in \mathbb{C}^{n \times n}$ $\mathbf{H} \in \mathbb{C}^{n \times n}$	$\begin{array}{lll} \mathbf{A} \in \mathbb{C}^{n \times n} & \mathbf{b} = \mathbf{A} \mathbf{x} \\ \mathbf{F} \in \mathbb{C}^{n \times n} & \mathbf{b} = \mathbf{F} \mathbf{x} \\ \mathbf{A}, \mathbf{B} \in \mathbb{C}^{n \times n} & \mathbf{c} = \mathbf{A} \mathbf{B} \\ \mathbf{A} \in \mathbb{C}^{n \times n} & \mathbf{A}^{-1} & \mathbf{A} \in \mathbb{C}^{n \times n} \\ \mathbf{A} \in \mathbb{C}^{n \times n} & \mathbf{H} = \mathbf{L} \mathbf{U} \\ \mathbf{H} \in \mathbb{C}^{n \times n} & \mathbf{H} = \mathbf{L} \mathbf{U} \\ \mathbf{H} \in \mathbb{C}^{n \times n} & \mathbf{H} = \mathbf{L} \mathbf{U} \\ \mathbf{A} \in \mathbb{C}^{n \times n} & \mathbf{A} = \mathbf{R}^* \mathbf{R} \\ \mathbf{L} \in \mathbb{C}^{n \times n} & \mathbf{L} \mathbf{x} = \mathbf{b} \\ \mathbf{L} \in \mathbb{C}^{n \times n} & \mathbf{L}^{-1} \\ \mathbf{A} \in \mathbb{C}^{m \times n} & \mathbf{A} \in \mathbb{C}^{m \times n} \\ \mathbf{A} \in \mathbb{C}^{m \times n} & \mathbf{A} \in \mathbb{C}^{m \times n} \\ \mathbf{A} \in \mathbb{C}^{n \times n} & \mathbf{B} = \mathbf{U}^* \mathbf{A} \mathbf{V} \\ \mathbf{A} \in \mathbb{C}^{n \times n} & \mathbf{H} = \mathbf{Q}^* \mathbf{A} \mathbf{Q} \\ \mathbf{T} = \mathbf{Q}^* \mathbf{A} \mathbf{Q} \end{array}$

Remark 2

On modern computer architectures the communication costs in moving data between different levels of memory or between processors in a network can exceed the arithmetic costs by orders of magnitude.

4. Circulant matrix

Definition 3

An $n \times n$ matrix **C** is called circulant if it has the form

$$\mathbf{C} = \begin{bmatrix} c_0 & c_{n-1} & \cdots & c_2 & c_1 \\ c_1 & c_0 & c_{n-1} & \ddots & c_2 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ c_{n-2} & \ddots & c_1 & c_0 & c_{n-1} \\ c_{n-1} & c_{n-2} & \cdots & c_1 & c_0 \end{bmatrix}.$$

We indicate this situation by $\mathbf{C} = \mathbf{circ}(\mathbf{c})$, where

$$\mathbf{c} = \begin{bmatrix} c_0 & c_1 & \cdots & c_{n-1} \end{bmatrix}^\top \in \mathbb{C}^n$$

• Discussion: How can you generate a circulant matrix in Matlab?

Definition 4

The $n \times n$ circulant right shift matrix is given by

$$\mathbf{R} = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix} = \mathbf{circ} \left(\begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \end{bmatrix}^{\mathsf{T}} \right).$$

• Obviously, if $\mathbf{C} = \mathbf{circ}(\mathbf{c})$, then $\mathbf{C} = \sum_{j=0}^{\infty} c_j \mathbf{R}^j$.

Lemma 5

Let
$$\omega_n = e^{-i2\pi/n}$$
. Then

$$\mathbf{R} = \frac{1}{n} \mathbf{F}_n^* \operatorname{diag}\{1, \omega_n, \omega_n^2, \cdots, \omega_n^{n-1}\} \mathbf{F}_n.$$

Theorem 6

If
$$C = circ(c)$$
, then

$$\mathbf{C} = \mathbf{F}_n^{-1} \operatorname{diag}\{\widehat{\mathbf{c}}\} \mathbf{F}_n = \frac{1}{n} \mathbf{F}_n^* \operatorname{diag}\{\widehat{\mathbf{c}}\} \mathbf{F}_n$$

where

$$\hat{\mathbf{c}} = \mathbf{F}_n \mathbf{c}$$
.

Fast algorithm 1: Circulant matrix-vector product $\mathbf{v} = \mathbf{C}\mathbf{u}$

- Step 1: Compute $\hat{\mathbf{c}} = \mathbf{F}_n \mathbf{c}$ and $\hat{\mathbf{u}} = \mathbf{F}_n \mathbf{u}$ by FFTs
- Step 2: Compute the component-wise vector product $\hat{\mathbf{v}} = \hat{\mathbf{c}} \cdot \hat{\mathbf{u}}$
- Step 3: Compute $\mathbf{v} = \frac{1}{n} \mathbf{F}_n^* \hat{\mathbf{v}}$ by iFFT

5. Toeplitz matrix

Definition 7

A matrix is called Toeplitz if it is constant along diagonals. An $n \times n$ Toeplitz matrix ${\bf T}$ has the form

$$\mathbf{T} = \begin{bmatrix} t_0 & t_{-1} & \cdots & t_{2-n} & t_{1-n} \\ t_1 & t_0 & t_{-1} & \ddots & t_{2-n} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ t_{n-2} & \ddots & t_1 & t_0 & t_{-1} \\ t_{n-1} & t_{n-2} & \cdots & t_1 & t_0 \end{bmatrix}.$$

We indicate this situation by $T = \mathbf{toep}(t)$, where

$$\mathbf{t} = \begin{bmatrix} t_{1-n} & \cdots & t_{-1} & t_0 & t_1 & \cdots & t_{n-1} \end{bmatrix}^\top \in \mathbb{C}^{2n-1}.$$

• Explore toeplitz(c,r) in Matlab.

• Define S = toep(s), where

$$\mathbf{s} = \begin{bmatrix} t_1 & t_2 & \cdots & t_{n-1} & 0 & t_{1-n} & \cdots & t_{-2} & t_{-1} \end{bmatrix}^{\top}.$$

Then we have

$$\mathbf{T}^{ce} := \begin{bmatrix} \mathbf{T} & \mathbf{S} \\ \mathbf{S} & \mathbf{T} \end{bmatrix} = \mathbf{circ}(\mathbf{t}^{ce}),$$

where

$$\mathbf{t}^{\mathrm{ce}} = \begin{bmatrix} t_0 & t_1 & \cdots & t_{n-1} & 0 & t_{1-n} & \cdots & t_{-2} & t_{-1} \end{bmatrix}^\top \in \mathbb{C}^{2n}.$$

Note that

$$\begin{bmatrix} \mathbf{T} & \mathbf{S} \\ \mathbf{S} & \mathbf{T} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{T}\mathbf{u} \\ \mathbf{S}\mathbf{u} \end{bmatrix}.$$

Using the fast algorithm for a circulant matrix-vector product, we obtain the following fast algorithm for a Toeplitz matrix-vector product $\mathbf{v} = \mathbf{T}\mathbf{u}$.

Fast algorithm 2: Toeplitz matrix-vector product $\mathbf{v} = \mathbf{T}\mathbf{u}$

Step 1: Compute $\widehat{\mathbf{t}^{ce}} = \mathbf{F}_{2n}\mathbf{t}^{ce}$ and $\widehat{\mathbf{u}^{ze}} = \mathbf{F}_{2n}[\mathbf{u}^{\top} \ \mathbf{0}]^{\top}$ by FFTs

Step 2: Compute the component-wise vector product $\hat{\mathbf{w}} = \hat{\mathbf{t}}^{ce}. * \hat{\mathbf{u}}^{ze}$

Step 3: Compute $\mathbf{w} = \frac{1}{2n} \mathbf{F}_{2n}^* \widehat{\mathbf{w}}$ by iFFT

Step 4: Extract the first n components of \mathbf{w} to obtain \mathbf{v} , i.e., $\mathbf{v} = \mathbf{w}(1:n)$

6. Hankel matrix

• A Hankel matrix $\mathbf{H} = \begin{bmatrix} h_{ij} \end{bmatrix}$ has identical elements along all its anti-diagonals, meaning that

$$h_{ij} = h_{i+l,j-l}$$

for all relevant integers i, j, and l.

• Explore hankel(c,r) in Matlab.

- A Hankel matrix is symmetric by definition.
- The relation to a Toeplitz matrix: the matrix

$$\mathbf{T} = \mathbf{JH}, \qquad \mathbf{J} = \begin{bmatrix} & & & 1 \\ & & 1 & \\ & \ddots & & \\ 1 & & & \end{bmatrix}$$

is a Toeplitz matrix, where \mathbf{J} is a permutation matrix obtained by reversing the columns (or rows) of the identity.

- Fast algorithm for a Hankel matrix-vector product can be obtained easily from that of a Toeplitz matrix-vector product.
- Other issue: Discrete cosine transform: dct symmetric Toeplitz-plus-Hankel (STH) matrix ...

7. Kronecker product and $vec(\cdot)$ operator

Definition 8

Let $\mathbf{A} \in \mathbb{C}^{m \times n}$ and $\mathbf{B} \in \mathbb{C}^{p \times q}$. Then $\mathbf{A} \otimes \mathbf{B}$, the Kronecker product of \mathbf{A} and \mathbf{B} , is the $mp \times nq$ matrix

$$\mathbf{A} \otimes \mathbf{B} := \begin{bmatrix} a_{11}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & \cdots & a_{mn}\mathbf{B} \end{bmatrix}.$$

Definition 9

Let $\mathbf{A} \in \mathbb{C}^{m \times n}$. Then $\text{vec}(\mathbf{A})$ is defined to be a column vector of size mn made of the columns of \mathbf{A} stacked atop one another from left to right.

• If $\mathbf{A} = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_n \end{bmatrix}$, then

$$\operatorname{vec}(\mathbf{A}) = egin{bmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \vdots \\ \mathbf{a}_n \end{bmatrix}.$$

• Let $\mathbf{A}, \mathbf{B} \in \mathbb{C}^{m \times n}$. Then $\operatorname{tr}(\mathbf{A}^* \mathbf{B}) = \operatorname{vec}(\mathbf{A})^* \operatorname{vec}(\mathbf{B})$.

Theorem 10

Let $\mathbf{A} \in \mathbb{C}^{p \times m}$, $\mathbf{X} \in \mathbb{C}^{m \times n}$ and $\mathbf{B} \in \mathbb{C}^{n \times q}$. Then the following properties hold

$$vec(\mathbf{AX}) = (\mathbf{I}_n \otimes \mathbf{A})vec(\mathbf{X}),$$
$$vec(\mathbf{XB}) = (\mathbf{B}^\top \otimes \mathbf{I}_m)vec(\mathbf{X}),$$
$$vec(\mathbf{AXB}) = (\mathbf{B}^\top \otimes \mathbf{A})vec(\mathbf{X}).$$

Theorem 11

The following facts about Kronecker products hold:

$$(\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}) = (\mathbf{AC}) \otimes (\mathbf{BD}),$$

$$(\mathbf{A} \otimes \mathbf{B})^{-1} = \mathbf{A}^{-1} \otimes \mathbf{B}^{-1},$$

$$(\mathbf{A} \otimes \mathbf{B})^{\dagger} = \mathbf{A}^{\dagger} \otimes \mathbf{B}^{\dagger},$$

$$(\mathbf{A} \otimes \mathbf{B})^{\top} = \mathbf{A}^{\top} \otimes \mathbf{B}^{\top}.$$

• Exercise: For $\mathbf{A} \in \mathbb{C}^{m \times n}$, $\mathbf{B} \in \mathbb{C}^{p \times q}$ and $\mathbf{C} \in \mathbb{C}^{m \times q}$, solve

$$\min_{\mathbf{X} \in \mathbb{C}^{n \times p}} \|\mathbf{A}\mathbf{X}\mathbf{B} - \mathbf{C}\|_{F} = ?$$

 \bullet Exercise: Let \mathcal{T} denote the triangular truncation operator, which is a linear operator that maps a given matrix to its strictly lower triangular part. Write down the matrix form of this operator.

• Exercise: Let $\mathbf{A} \in \mathbb{C}^{m \times m}$ and $\mathbf{B} \in \mathbb{C}^{n \times n}$. What are eigenvalues of

$$\mathbf{I} \otimes \mathbf{A} + \mathbf{B} \otimes \mathbf{I}$$

and

$$\mathbf{A} \otimes \mathbf{B}$$
?

8. Reference books for Toeplitz solver and FFT

- Chan, Raymond Hon-Fu and Jin, Xiao-Qing
 An introduction to iterative Toeplitz solvers, SIAM, 2007
- Van Loan, Charles
 Computational frameworks for the fast Fourier transform, SIAM, 1992