Algorithms of Scientific Computing

Discrete Fourier Transform (DFT)

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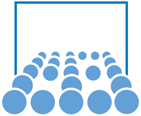

Fast Fourier Transform – Outline

- Discrete Fourier transform
- Fast Fourier transform
- Special Fourier transform:
  - real-valued FFT
  - sine/cosine transform
- Applications:
  - Fast Poisson solver (FST)
  - Computergraphics (FCT)
- Efficient Implementation

Discrete Fourier Transform (DFT)

Definition:
For a vector of N complex numbers $(f_0, \ldots, f_{N-1})$, the **discrete Fourier transform** is given by the vector $(F_0, \ldots, F_{N-1})$, where

$$F_k = \frac{1}{N} \sum_{n=0}^{N-1} f_n e^{-i2\pi nk/N}.$$

Interpretation:

- as trigonometric interpolation/approxmiation
- as approximation of the coefficients of the Fourier series

DFT as Interpolation (1)

Interpolation problem:

- N ansatz functions: $g_k(x) := e^{ikx}$ in the interval $[0, 2\pi]$, $k = 0, \ldots, N-1$
- N supporting points: $x_n := 2\pi n/N$, $n = 0, \ldots, N-1$
- N interpolation value f_n, $n = 0, \ldots, N-1$
- find N weights F_k such that at all supporting points

$$f_n = \sum_{k=0}^{N-1} F_k g_k(x_n) \qquad \Leftrightarrow \qquad f_n = \sum_{k=0}^{N-1} F_k e^{i2\pi nk/N}.$$

”trigonometric interpolation”

DFT as Interpolation (2)

Interpolation problem:

- N ansatz functions: $\widetilde{g}_k(z) := z^k$ (complex unit polynomials), $k = 0, \ldots, N-1$
- N supporting points: $z_n := e^{i2\pi n/N} = \omega_N^n$, where $\omega_N := e^{i2\pi/N}$
- N interpolation values f_n, $n = 0, \ldots, N-1$, respectively.
- find the N weights F_k such that at all supporting points

$$f_n = \sum_{k=0}^{N-1} F_k \widetilde{g}_k(z_n) \qquad \Leftrightarrow \qquad f_n = \sum_{k=0}^{N-1} F_k e^{i2\pi nk/N}.$$

Polynomial interpolation at the "complex unit roots"ω_N^n

Interpretation of the Interpolation Problem

Starting from the first formulation,

$$f_n = \sum_{k=0}^{N-1} F_k g_k(x_n), \qquad g_k(x_n) = e^{i2\pi nk/N},$$

we look for a representation of the signal f_n – or of a function $f(x)$ – of the form

$$f(x) = \sum_{k=0}^{N-1} F_k g_k(x), \qquad g_k(x) = e^{i2\pi kx}.$$

The ansatz functions are sine or cosine oscillations:

$$e^{ikx} = \cos(kx) + i\sin(kx)$$

Interpretation of the Interpolation Problem (2)

Conclusions:

- we look for the **representation of a periodic function** as a sum of sines and cosines
- the F_k are, thus, called **Fourier coefficients**:
  - k represents the wave number
  - the value of F_k represents the amplitude of the corresponding frequency
- the Fourier transform leads to a **frequency spectrum**
- useful when a problem is easier to solve in the **frequency domain** than in the **spatial domain**.

Solution of the Interpolation Problem

Both interpolation problems lead to the identical linear systems of equations:

$$f_n = \sum_{k=0}^{N-1} F_k \omega_N^{nk}, \quad \text{for all } n = 0, \ldots, N-1;$$

where $\omega_N := e^{i2\pi/N}$, i.e. $\omega_N^{nk} := e^{i2\pi nk/N}$.

If we write the vectors of the f_n and F_k as $\mathbf{f} := (f_0, \ldots, f_{N-1})$ and $\mathbf{F} := (F_0, \ldots, F_{N-1})$, the linear system of equations can be formulated in matrix-vector notation

$$\mathbf{WF} = \mathbf{f},$$

where the entries of the matrix $\mathbf{W}$ are given by $W_{nk} := \omega_N^{nk}$.

Properties of the Matrix W

- $\mathbf{W}$ is symmetric: $\mathbf{W} = \mathbf{W}^T$, and has the form

$$\mathbf{W} = \begin{pmatrix} \omega_N^0 & \omega_N^0 & \omega_N^0 & \dots & \omega_N^0 \\ \omega_N^0 & \omega_N^1 & \omega_N^2 & \dots & \omega_N^{(N-1)} \\ \omega_N^0 & \omega_N^2 & \omega_N^4 & \dots & \omega_N^{2(N-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ \omega_N^0 & \omega_N^{(N-1)} & \omega_N^{2(N-1)} & \dots & \omega_N^{(N-1)(N-1)} \end{pmatrix}$$

- $\mathbf{W}\left(\mathbf{W}^T\right)^* = \mathbf{W}\mathbf{W}^H = N\mathbf{I}$, since

$$\left[\mathbf{W}\mathbf{W}^H\right]_{kl} = \sum_{j=0}^{N-1} \omega_N^{kj}\left(\omega_N^{lj}\right)^* = \sum_{j=0}^{N-1} \omega_N^{(k-l)j} = \begin{cases} N & \text{if} \quad k = l \\ 0 & \text{if} \quad k \neq l. \end{cases}$$

Computation of the Fourier Coefficients F_k

- Since $\mathbf{W}\mathbf{W}^H = N\mathbf{I}$, $\mathbf{W}^{-1} = \frac{1}{N}\mathbf{W}^H$ holds, resulting in

$$\mathbf{W}^{-1} = \frac{1}{N}\begin{pmatrix} \omega_N^0 & \omega_N^0 & \omega_N^0 & \dots & \omega_N^0 \\ \omega_N^0 & \omega_N^{-1} & \omega_N^{-2} & \dots & \omega_N^{-(N-1)} \\ \omega_N^0 & \omega_N^{-2} & \omega_N^{-4} & \dots & \omega_N^{-2(N-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ \omega_N^0 & \omega_N^{-(N-1)} & \omega_N^{-2(N-1)} & \dots & \omega_N^{-(N-1)(N-1)} \end{pmatrix}$$

⇒ the vector **F** of the Fourier coefficients can be computed **easily** as a matrix-vector product – with computational effort $\mathcal{O}(N^2)$:

$$\mathbf{F} = \frac{1}{N}\mathbf{W}^H\mathbf{f} \qquad \text{or} \qquad F_k = \frac{1}{N}\sum_{n=0}^{N-1} f_n \omega_N^{-nk}.$$

Inverse Discrete Fourier Transform (IDFT)

Definition: The inverse Discrete Fourier Transform (IDFT) of the vector $(F_0, \ldots, F_{N-1})$ is given by the vector $(f_0, \ldots, f_{N-1})$, where

$$f_n = \sum_{k=0}^{N-1} F_k e^{i2\pi nk/N}.$$

Observation:
DFT and IDFT are inverse operations:

$$F_k = \frac{1}{N} \sum_{n=0}^{N-1} f_n e^{-i2\pi nk/N} , \qquad f_n = \sum_{k=0}^{N-1} F_k e^{i2\pi nk/N} .$$

$$\mathbf{F} = \mathrm{DFT}(\mathrm{IDFT}(\mathbf{F})) \quad \text{or} \quad \mathbf{f} = \mathrm{IDFT}(\mathrm{DFT}(\mathbf{f})).$$

The Pair DFT/IDFT as Matrix-Vector Product

With the notation $\omega_N := e^{i2\pi/N}$, i.e. ${\omega_N}^{-nk} := e^{-i2\pi nk/N}$, we formulate DFT/IDFT as

$$F_k = \frac{1}{N}\sum_{n=0}^{N-1} f_n {\omega_N}^{-nk} \qquad f_n = \sum_{k=0}^{N-1} F_k \omega_N^{nk}$$

With the vectors $\mathbf{f} := (f_0, \ldots, f_{N-1})$ and $\mathbf{F} := (F_0, \ldots, F_{N-1})$, we denote (and compute) the DFT und IDFT as matrix-vector products

$$\mathbf{F} = \frac{1}{N}\mathbf{W}^H\mathbf{f}\,, \qquad \mathbf{f} = \mathbf{WF}\,,$$

where the elements of the matrix **W** are given by $W_{nk} := \omega_N^{nk}$.

Properties of the DFT

- DFT and IDFT are (as a matrix-vector product) **linear**:

$$\begin{aligned}\mathrm{DFT}(\alpha f + \beta g) &= \alpha\,\mathrm{DFT}(f) + \beta\,\mathrm{DFT}(g)\\ \mathrm{IDFT}(\alpha f + \beta g) &= \alpha\,\mathrm{IDFT}(f) + \beta\,\mathrm{IDFT}(g)\end{aligned}$$

- since $\omega_N^{nk} = \omega_N^{n(k+N)} = \omega_N^{(n+N)k}$, the f_n and the F_k are **periodic**:

$$f_{n+N} = f_n \qquad F_{k+N} = F_k \qquad \text{for all } k, n \in \mathbb{Z}$$

Alternative Forms of the DFT

Possible variants (in all imaginable combinations):

- Scaling factor $\frac{1}{N}$ in the IDFT instead of the DFT; alternatively a factor $\frac{1}{\sqrt{N}}$ in DFT and IDFT.
- switched signs in the exponent of the exponential function in DFT and IDFT
- use *j* for the imaginary unit (electrical engineering)

Shift of indices:

- periodic data: $F_k = F_{k+N}$
- aliasing of frequencies: $e^{-i2\pi nk/N} = e^{-i2\pi n(k\pm N)/N}$

DFT with Shifted Indices

Data and frequencies "symmetric":

$$F_k = \frac{1}{N} \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} f_n e^{-i2\pi nk/N}\,, \qquad f_n = \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} F_k e^{i2\pi nk/N}$$

In general:

$$F_k = \frac{1}{N} \sum_{n=P+1}^{P+N} f_n e^{-i2\pi nk/N}\,, \qquad f_n = \sum_{k=Q+1}^{Q+N} F_k e^{i2\pi nk/N}$$

DFT in Program Libraries

Matlab, IMSL (Int. Math. and Stat. Library):

$$
\begin{aligned}
F_{k+1} &= \sum_{n=0}^{N-1} f_{n+1} e^{-i2\pi nk/N} \qquad && k = 0, \ldots, N-1 \\
f_{n+1} &= \frac{1}{N} \sum_{k=0}^{N-1} F_{k+1} e^{i2\pi nk/N} \qquad && n = 0, \ldots, N-1
\end{aligned}
$$

Maple: $\frac{1}{\sqrt{N}}$ as factor for DFT and IDFT.

Index shift by $+1$, since:

- Data/coefficients start at index 0
- Arrays to store the numbers start at index 1