

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

1.3.2.7.4. Matrix representation of the discrete Fourier transform (DFT)

By virtue of definitions (i) and (ii),

$$\begin{aligned}\mathcal{F}(\mathbf{N})\mathbf{v}_{k^*} &= \frac{1}{|\det \mathbf{N}|} \sum_k \exp[-2\pi i k^* \cdot (\mathbf{N}^{-1}k)] \mathbf{u}_k \\ \tilde{\mathcal{F}}(\mathbf{N})\mathbf{u}_k &= \sum_{k^*} \exp[+2\pi i k^* \cdot (\mathbf{N}^{-1}k)] \mathbf{v}_{k^*}\end{aligned}$$

so that $\mathcal{F}(\mathbf{N})$ and $\tilde{\mathcal{F}}(\mathbf{N})$ may be represented, in the canonical bases of $W_{\mathbf{N}}$ and $W_{\mathbf{N}}^*$, by the following matrices:

$$\begin{aligned}[\mathcal{F}(\mathbf{N})]_{kk^*} &= \frac{1}{|\det \mathbf{N}|} \exp[-2\pi i k^* \cdot (\mathbf{N}^{-1}k)] \\ [\tilde{\mathcal{F}}(\mathbf{N})]_{k^*k} &= \exp[+2\pi i k^* \cdot (\mathbf{N}^{-1}k)].\end{aligned}$$

When \mathbf{N} is symmetric, $\mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n$ and $\mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n$ may be identified in a natural manner, and the above matrices are symmetric.

When \mathbf{N} is diagonal, say $\mathbf{N} = \text{diag}(\nu_1, \nu_2, \dots, \nu_n)$, then the tensor product structure of the full multidimensional Fourier transform (Section 1.3.2.4.2.4)

$$\mathcal{F}_{\mathbf{x}} = \mathcal{F}_{x_1} \otimes \mathcal{F}_{x_2} \otimes \dots \otimes \mathcal{F}_{x_n}$$

gives rise to a tensor product structure for the DFT matrices. The tensor product of matrices is defined as follows:

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} a_{11}\mathbf{B} & \dots & a_{1n}\mathbf{B} \\ \vdots & & \vdots \\ a_{n1}\mathbf{B} & \dots & a_{nn}\mathbf{B} \end{pmatrix}.$$

Let the index vectors k and k^* be ordered in the same way as the elements in a Fortran array, e.g. for k with k_1 increasing fastest, k_2 next fastest, ..., k_n slowest; then

$$\mathcal{F}(\mathbf{N}) = \mathcal{F}(\nu_1) \otimes \mathcal{F}(\nu_2) \otimes \dots \otimes \mathcal{F}(\nu_n),$$

where

$$[\mathcal{F}(\nu_j)]_{k_j, k_j^*} = \frac{1}{\nu_j} \exp\left(-2\pi i \frac{k_j^* k_j}{\nu_j}\right),$$

and

$$\tilde{\mathcal{F}}(\mathbf{N}) = \tilde{\mathcal{F}}(\nu_1) \otimes \tilde{\mathcal{F}}(\nu_2) \otimes \dots \otimes \tilde{\mathcal{F}}(\nu_n),$$

where

$$[\tilde{\mathcal{F}}(\nu_j)]_{k_j^*, k_j} = \exp\left(+2\pi i \frac{k_j^* k_j}{\nu_j}\right).$$

1.3.2.7.5. Properties of the discrete Fourier transform

The DFT inherits most of the properties of the Fourier transforms, but with certain numerical factors ('Jacobians') due to the transition from continuous to discrete measure.

(1) *Linearity* is obvious.

(2) *Shift property*. If $(\tau_a \psi)(k) = \psi(k - a)$ and $(\tau_a \Psi)(k^*) = \Psi(k^* - a^*)$, where subtraction takes place by modular vector arithmetic in $\mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n$ and $\mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n$, respectively, then the following identities hold:

$$\begin{aligned}\tilde{\mathcal{F}}(\mathbf{N})[\tau_a \psi](k^*) &= \exp[+2\pi i k^* \cdot (\mathbf{N}^{-1}a)] \tilde{\mathcal{F}}(\mathbf{N})[\psi](k^*) \\ \mathcal{F}(\mathbf{N})[\tau_a \Psi](k) &= \exp[-2\pi i k \cdot (\mathbf{N}^{-1}a)] \mathcal{F}(\mathbf{N})[\Psi](k).\end{aligned}$$

(3) *Differentiation identities*. Let vectors ψ and Ψ be constructed from $\varphi^0 \in \mathcal{E}(\mathbb{R}^n)$ as in Section 1.3.2.7.3, hence be related by the DFT. If $D^{\mathbf{p}}\psi$ designates the vector of sample values of $D_{\mathbf{x}}^{\mathbf{p}}\varphi^0$ at the points of $\Lambda_{\mathbf{B}}/\Lambda_{\mathbf{A}}$, and $D^{\mathbf{p}}\Psi$ the vector of values of $D_{\xi}^{\mathbf{p}}\Phi^0$ at points of

$\Lambda_{\mathbf{A}}^*/\Lambda_{\mathbf{B}}^*$, then for all multi-indices $\mathbf{p} = (p_1, p_2, \dots, p_n)$

$$\begin{aligned}(D^{\mathbf{p}}\psi)(k) &= \tilde{\mathcal{F}}(\mathbf{N})[(+2\pi i k^*)^{\mathbf{p}}\Psi](k) \\ (D^{\mathbf{p}}\Psi)(k^*) &= \mathcal{F}(\mathbf{N})[(-2\pi i k)^{\mathbf{p}}\psi](k^*)\end{aligned}$$

or equivalently

$$\begin{aligned}\tilde{\mathcal{F}}(\mathbf{N})[D^{\mathbf{p}}\psi](k^*) &= (+2\pi i k^*)^{\mathbf{p}}\Psi(k^*) \\ \mathcal{F}(\mathbf{N})[D^{\mathbf{p}}\Psi](k) &= (-2\pi i k)^{\mathbf{p}}\psi(k).\end{aligned}$$

(4) *Convolution property*. Let $\varphi \in W_{\mathbf{N}}$ and $\Phi \in W_{\mathbf{N}}^*$ (respectively ψ and Ψ) be related by the DFT, and define

$$\begin{aligned}(\varphi * \psi)(k) &= \sum_{k' \in \mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n} \varphi(k') \psi(k - k') \\ (\Phi * \Psi)(k^*) &= \sum_{k' \in \mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n} \Phi(k') \Psi(k^* - k').\end{aligned}$$

Then

$$\begin{aligned}\tilde{\mathcal{F}}(\mathbf{N})[\Phi * \Psi](k) &= |\det \mathbf{N}| \varphi(k) \psi(k) \\ \mathcal{F}(\mathbf{N})[\varphi * \psi](k^*) &= \Phi(k^*) \Psi(k^*)\end{aligned}$$

and

$$\begin{aligned}\tilde{\mathcal{F}}(\mathbf{N})[\varphi \times \psi](k^*) &= \frac{1}{|\det \mathbf{N}|} (\Phi * \Psi)(k^*) \\ \mathcal{F}(\mathbf{N})[\Phi \times \Psi](k) &= (\varphi * \psi)(k).\end{aligned}$$

Since addition on $\mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n$ and $\mathbb{Z}^n/\mathbf{N}^T\mathbb{Z}^n$ is modular, this type of convolution is called *cyclic convolution*.

(5) *Parseval/Plancherel property*. If $\varphi, \psi, \Phi, \Psi$ are as above, then

$$\begin{aligned}(\mathcal{F}(\mathbf{N})[\Phi], \mathcal{F}(\mathbf{N})[\Psi])_W &= \frac{1}{|\det \mathbf{N}|} (\Phi, \Psi)_{W^*} \\ (\tilde{\mathcal{F}}(\mathbf{N})[\varphi], \tilde{\mathcal{F}}(\mathbf{N})[\psi])_W &= \frac{1}{|\det \mathbf{N}|} (\varphi, \psi)_W.\end{aligned}$$

(6) *Period 4*. When \mathbf{N} is symmetric, so that the ranges of indices k and k^* can be identified, it makes sense to speak of powers of $\mathcal{F}(\mathbf{N})$ and $\tilde{\mathcal{F}}(\mathbf{N})$. Then the 'standardized' matrices $(1/|\det \mathbf{N}|^{1/2})\mathcal{F}(\mathbf{N})$ and $(1/|\det \mathbf{N}|^{1/2})\tilde{\mathcal{F}}(\mathbf{N})$ are *unitary* matrices whose fourth power is the identity matrix (Section 1.3.2.4.3.4); their eigenvalues are therefore ± 1 and $\pm i$.

1.3.3. Numerical computation of the discrete Fourier transform

1.3.3.1. Introduction

The Fourier transformation's most remarkable property is undoubtedly that of turning convolution into multiplication. As distribution theory has shown, other valuable properties – such as the shift property, the conversion of differentiation into multiplication by monomials, and the duality between periodicity and sampling – are special instances of the convolution theorem.

This property is exploited in many areas of applied mathematics and engineering (Campbell & Foster, 1948; Sneddon, 1951; Champeney, 1973; Bracewell, 1986). For example, the passing of a signal through a linear filter, which results in its being convolved with the response of the filter to a δ -function 'impulse', may be modelled as a multiplication of the signal's transform by the transform of the impulse response (also called transfer function). Similarly, the solution of systems of partial differential equations may be turned by Fourier transformation into a division problem for distributions. In both cases, the formulations obtained after Fourier transformation are considerably simpler than the initial ones, and lend themselves to constructive solution techniques.