

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

B is a diagonal matrix of multiplications,

C is a matrix with entries 0, ±1, ±i, defining the ‘post-additions’.

The elements on the diagonal of **B** can be shown to be either real or pure imaginary, by the same argument as in Section 1.3.3.2.3.1. Matrices **A** and **C** may be rectangular rather than square, so that intermediate results may require extra storage space.

1.3.3.3. *Multidimensional algorithms*

From an algorithmic point of view, the distinction between one-dimensional (1D) and multidimensional DFTs is somewhat blurred by the fact that some factoring techniques turn a 1D transform into a multidimensional one. The distinction made here, however, is a practical one and is based on the dimensionality of the indexing sets for data and results. This section will therefore be concerned with the problem of factoring the DFT when the *indexing sets* for the input data and output results are multidimensional.

1.3.3.3.1. *The method of successive one-dimensional transforms*

The DFT was defined in Section 1.3.2.7.4 in an *n*-dimensional setting and it was shown that when the decimation matrix **N** is diagonal, say $\mathbf{N} = \text{diag}(N^{(1)}, N^{(2)}, \dots, N^{(n)})$, then $\bar{F}(N)$ has a tensor product structure:

$$\bar{F}(\mathbf{N}) = \bar{F}(N^{(1)}) \otimes \bar{F}(N^{(2)}) \otimes \dots \otimes \bar{F}(N^{(n)}).$$

This may be rewritten as follows:

$$\begin{aligned} \bar{F}(\mathbf{N}) &= [\bar{F}(N^{(1)}) \otimes I_{N^{(2)}} \otimes \dots \otimes I_{N^{(n)}}] \\ &\times [I_{N^{(1)}} \otimes \bar{F}(N^{(2)}) \otimes \dots \otimes I_{N^{(n)}}] \\ &\times \dots \\ &\times [I_{N^{(1)}} \otimes I_{N^{(2)}} \otimes \dots \otimes \bar{F}(N^{(n)})], \end{aligned}$$

where the *I*'s are identity matrices and × denotes ordinary matrix multiplication. The matrix within each bracket represents a one-dimensional DFT along one of the *n* dimensions, the other dimensions being left untransformed. As these matrices commute, the order in which the successive 1D DFTs are performed is immaterial.

This is the most straightforward method for building an *n*-dimensional algorithm from existing 1D algorithms. It is known in crystallography under the name of ‘Beavers–Lipson factorization’ (Section 1.3.4.3.1), and in signal processing as the ‘row–column method’.

1.3.3.3.2. *Multidimensional factorization*

Substantial reductions in the arithmetic cost, as well as gains in flexibility, can be obtained if the factoring of the DFT is carried out in several dimensions simultaneously. The presentation given here is a generalization of that of Mersereau & Speake (1981), using the abstract setting established independently by Auslander, Tolimieri & Winograd (1982).

Let us return to the general *n*-dimensional setting of Section 1.3.2.7.4, where the DFT was defined for an arbitrary decimation matrix **N** by the formulae (where |**N**| denotes |det **N**|):

$$\begin{aligned} F(\mathbf{N}) : \quad X(\mathbf{k}) &= \frac{1}{|\mathbf{N}|} \sum_{\mathbf{k}^*} X^*(\mathbf{k}^*) e[-\mathbf{k}^* \cdot (\mathbf{N}^{-1}\mathbf{k})] \\ \bar{F}(\mathbf{N}) : \quad X^*(\mathbf{k}^*) &= \sum_{\mathbf{k}} X(\mathbf{k}) e[\mathbf{k}^* \cdot (\mathbf{N}^{-1}\mathbf{k})] \end{aligned}$$

with

$$\mathbf{k} \in \mathbb{Z}^n / \mathbf{N}\mathbb{Z}^n, \quad \mathbf{k}^* \in \mathbb{Z}^n / \mathbf{N}^T \mathbb{Z}^n.$$

1.3.3.3.2.1. *Multidimensional Cooley–Tukey factorization*

Let us now assume that this decimation can be factored into *d* successive decimations, *i.e.* that

$$\mathbf{N} = \mathbf{N}_1 \mathbf{N}_2 \dots \mathbf{N}_{d-1} \mathbf{N}_d$$

and hence

$$\mathbf{N}^T = \mathbf{N}_d^T \mathbf{N}_{d-1}^T \dots \mathbf{N}_2^T \mathbf{N}_1^T.$$

Then the coset decomposition formulae corresponding to these successive decimations (Section 1.3.2.7.1) can be combined as follows:

$$\begin{aligned} \mathbb{Z}^n &= \bigcup_{\mathbf{k}_1} (\mathbf{k}_1 + \mathbf{N}_1 \mathbb{Z}^n) \\ &= \bigcup_{\mathbf{k}_1} \left\{ \mathbf{k}_1 + \mathbf{N}_1 \left[\bigcup_{\mathbf{k}_2} (\mathbf{k}_2 + \mathbf{N}_2 \mathbb{Z}^n) \right] \right\} \\ &= \dots \\ &= \bigcup_{\mathbf{k}_1} \dots \bigcup_{\mathbf{k}_d} (\mathbf{k}_1 + \mathbf{N}_1 \mathbf{k}_2 + \dots + \mathbf{N}_1 \mathbf{N}_2 \times \dots \times \mathbf{N}_{d-1} \mathbf{k}_d + \mathbf{N} \mathbb{Z}^n) \end{aligned}$$

with $\mathbf{k}_j \in \mathbb{Z}^n / \mathbf{N}_j \mathbb{Z}^n$. Therefore, any $\mathbf{k} \in \mathbb{Z} / \mathbf{N} \mathbb{Z}^n$ may be written uniquely as

$$\mathbf{k} = \mathbf{k}_1 + \mathbf{N}_1 \mathbf{k}_2 + \dots + \mathbf{N}_1 \mathbf{N}_2 \times \dots \times \mathbf{N}_{d-1} \mathbf{k}_d.$$

Similarly:

$$\begin{aligned} \mathbb{Z}^n &= \bigcup_{\mathbf{k}_d^*} (\mathbf{k}_d^* + \mathbf{N}_d^T \mathbb{Z}^n) \\ &= \dots \\ &= \bigcup_{\mathbf{k}_d^*} \dots \bigcup_{\mathbf{k}_1^*} (\mathbf{k}_d^* + \mathbf{N}_d^T \mathbf{k}_{d-1}^* + \dots + \mathbf{N}_d^T \times \dots \times \mathbf{N}_2^T \mathbf{k}_1^* + \mathbf{N}^T \mathbb{Z}^n) \end{aligned}$$

so that any $\mathbf{k}^* \in \mathbb{Z}^n / \mathbf{N}^T \mathbb{Z}^n$ may be written uniquely as

$$\mathbf{k}^* = \mathbf{k}_d^* + \mathbf{N}_d^T \mathbf{k}_{d-1}^* + \dots + \mathbf{N}_d^T \times \dots \times \mathbf{N}_2^T \mathbf{k}_1^*$$

with $\mathbf{k}_j^* \in \mathbb{Z}^n / \mathbf{N}_j^T \mathbb{Z}^n$. These decompositions are the vector analogues of the multi-radix number representation systems used in the Cooley–Tukey factorization.

We may then write the definition of $\bar{F}(\mathbf{N})$ with *d* = 2 factors as

$$\begin{aligned} X^*(\mathbf{k}_2^* + \mathbf{N}_2^T \mathbf{k}_1^*) &= \sum_{\mathbf{k}_1} \sum_{\mathbf{k}_2} X(\mathbf{k}_1 + \mathbf{N}_1 \mathbf{k}_2) \\ &\times e[(\mathbf{k}_2^{*T} + \mathbf{k}_1^{*T} \mathbf{N}_2) \mathbf{N}_2^{-1} \mathbf{N}_1^{-1} (\mathbf{k}_1 + \mathbf{N}_1 \mathbf{k}_2)]. \end{aligned}$$

The argument of *e*(–) may be expanded as

$$\mathbf{k}_2^* \cdot (\mathbf{N}_1^{-1} \mathbf{k}_1) + \mathbf{k}_1^* \cdot (\mathbf{N}_1^{-1} \mathbf{k}_1) + \mathbf{k}_2^* \cdot (\mathbf{N}_2^{-1} \mathbf{k}_2) + \mathbf{k}_1^* \cdot \mathbf{k}_2.$$

The first summand may be recognized as a twiddle factor, the second and third as the kernels of $\bar{F}(\mathbf{N}_1)$ and $\bar{F}(\mathbf{N}_2)$, respectively, while the fourth is an integer which may be dropped. We are thus led to a ‘vector-radix’ version of the Cooley–Tukey algorithm, in which the successive decimations may be introduced in all *n* dimensions simultaneously by general integer matrices. The computation may be decomposed into five stages analogous to those of the one-dimensional algorithm of Section 1.3.3.2.1:

(i) form the |**N**₁| vectors **Y**_{**k**₁} of shape **N**₂ by

$$Y_{\mathbf{k}_1}(\mathbf{k}_2) = X(\mathbf{k}_1 + \mathbf{N}_1 \mathbf{k}_2), \quad \mathbf{k}_1 \in \mathbb{Z}^n / \mathbf{N}_1 \mathbb{Z}^n, \quad \mathbf{k}_2 \in \mathbb{Z}^n / \mathbf{N}_2 \mathbb{Z}^n;$$