

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

$$\left(\bigotimes_{\gamma=1}^{\mu} \mathbf{C}_{\gamma} \right) \times \left(\bigotimes_{\beta=1}^{\mu} \mathbf{B}_{\beta} \right) \times \left(\bigotimes_{\alpha=1}^{\mu} \mathbf{A}_{\alpha} \right)$$

and thus to form a matrix in which the *combined* pre-addition, multiplication and post-addition matrices have been *precomputed*. This procedure, called *nesting*, can be shown to afford a reduction of the arithmetic operation count compared to the row–column method (Morris, 1978).

Clearly, the nesting rearrangement need not be applied to all μ dimensions, but can be restricted to any desired subset of them.

1.3.3.3.2.4. *The Nussbaumer–Quandalle algorithm*

Nussbaumer’s approach views the DFT as the evaluation of certain polynomials constructed from the data (as in Section 1.3.3.2.4). For instance, putting $\omega = e(1/N)$, the 1D N -point DFT

$$X^*(k^*) = \sum_{k=0}^{N-1} X(k)\omega^{k^*k}$$

may be written

$$X^*(k^*) = Q(\omega^{k^*}),$$

where the polynomial Q is defined by

$$Q(z) = \sum_{k=0}^{N-1} X(k)z^k.$$

Let us consider (Nussbaumer & Quandalle, 1979) a 2D transform of size $N \times N$:

$$X^*(k_1^*, k_2^*) = \sum_{k_1=0}^{N-1} \sum_{k_2=0}^{N-1} X(k_1, k_2)\omega^{k_1^*k_1+k_2^*k_2}.$$

By introduction of the polynomials

$$Q_{k_2}(z) = \sum_{k_1} X(k_1, k_2)z^{k_1}$$

$$R_{k_2^*}(z) = \sum_{k_2} \omega^{k_2^*k_2} Q_{k_2}(z),$$

this may be rewritten:

$$X^*(k_1^*, k_2^*) = R_{k_2^*}(\omega^{k_1^*}) = \sum_{k_2} \omega^{k_2^*k_2} Q_{k_2}(\omega^{k_1^*}).$$

Let us now suppose that k_1^* is coprime to N . Then k_1^* has a unique inverse modulo N (denoted by $1/k_1^*$), so that multiplication by k_1^* simply permutes the elements of $\mathbb{Z}/N\mathbb{Z}$ and hence

$$\sum_{k_2=0}^{N-1} f(k_2) = \sum_{k_2=0}^{N-1} f(k_1^*k_2)$$

for any function f over $\mathbb{Z}/N\mathbb{Z}$. We may thus write:

$$X^*(k_1^*, k_2^*) = \sum_{k_2} \omega^{k_1^*k_2^*k_2} Q_{k_1^*k_2}(\omega^{k_1^*})$$

$$= S_{k_1^*k_2}(\omega^{k_1^*})$$

where

$$S_{k^*}(z) = \sum_{k_2} z^{k^*k_2} Q_{k_2}(z).$$

Since only the value of polynomial $S_{k^*}(z)$ at $z = \omega^{k_1^*}$ is involved in the result, the computation of S_{k^*} may be carried out modulo the unique cyclotomic polynomial $P(z)$ such that $P(\omega^{k_1^*}) = 0$. Thus, if we define:

$$T_{k^*}(z) = \sum_{k_2} z^{k^*k_2} Q_{k_2}(z) \text{ mod } P(z)$$

we may write:

$$X^*(k_1^*, k_2^*) = T_{k_1^*k_2^*}(\omega^{k_1^*})$$

or equivalently

$$X^*\left(k_1^*, \frac{k_2^*}{k_1^*}\right) = T_{k_2^*}(\omega^{k_1^*}).$$

For N an odd prime p , all non-zero values of k_1^* are coprime with p so that the $p \times p$ -point DFT may be calculated as follows:

(1) form the polynomials

$$T_{k_2^*}(z) = \sum_{k_1} \sum_{k_2} X(k_1, k_2)z^{k_1+k_2^*k_2} \text{ mod } P(z)$$

for $k_2^* = 0, \dots, p-1$;

(2) evaluate $T_{k_2^*}(\omega^{k_1^*})$ for $k_1^* = 0, \dots, p-1$;

(3) put $X^*(k_1^*, k_2^*/k_1^*) = T_{k_2^*}(\omega^{k_1^*})$;

(4) calculate the terms for $k_1^* = 0$ separately by

$$X^*(0, k_2^*) = \sum_{k_1} \left[\sum_{k_2} X(k_1, k_2) \right] \omega^{k_2^*k_2}.$$

Step (1) is a set of p ‘polynomial transforms’ involving no multiplications; step (2) consists of p DFTs on p points each since if

$$T_{k_2^*}(z) = \sum_{k_1} Y_{k_2^*}(k_1)z^{k_1}$$

then

$$T_{k_2^*}(\omega^{k_1^*}) = \sum_{k_1} Y_{k_2^*}(k_1)\omega^{k_1^*k_1} = Y_{k_2^*}^*(k_1^*);$$

step (3) is a permutation; and step (4) is a p -point DFT. Thus the 2D DFT on $p \times p$ points, which takes $2p$ p -point DFTs by the row–column method, involves only $(p+1)$ p -point DFTs; the other DFTs have been replaced by polynomial transforms involving only additions.

This procedure can be extended to n dimensions, and reduces the number of 1D p -point DFTs from np^{n-1} for the row–column method to $(p^n - 1)/(p - 1)$, at the cost of introducing extra additions in the polynomial transforms.

A similar algorithm has been formulated by Auslander *et al.* (1983) in terms of Galois theory.

1.3.3.3.3. *Global algorithm design*

1.3.3.3.3.1. *From local pieces to global algorithms*

The mathematical analysis of the structure of DFT computations has brought to light a broad variety of possibilities for reducing or reshaping their arithmetic complexity. All of them are ‘analytic’ in that they break down large transforms into a succession of smaller ones.

These results may now be considered from the converse ‘synthetic’ viewpoint as providing a list of procedures for assembling them:

(i) the building blocks are one-dimensional p -point algorithms for p a small prime;

(ii) the low-level connectors are the multiplicative reindexing methods of Rader and Winograd, or the polynomial transform reindexing method of Nussbaumer and Quandalle, which allow the construction of efficient algorithms for larger primes p , for prime powers p^ν , and for p -primary pieces of shape $p^\nu \times \dots \times p^\nu$;

(iii) the high-level connectors are the additive reindexing scheme of Cooley–Tukey, the Chinese remainder theorem reindexing, and the tensor product construction;

(iv) nesting may be viewed as the ‘glue’ which seals all elements.