

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

(iv) calculate the N_2 transforms $\mathbf{Z}_{k_2}^*$ on N_1 points:

$$\mathbf{Z}_{k_2}^* = \bar{F}(N_1)[\mathbf{Z}_{k_2}^*], \quad k_2 \in \mathbb{Z}/N_2\mathbb{Z};$$

(v) collect $X^*(k_2^* + k_1^*N_2)$ as $Z_{k_1}^*(k_1^*)$.

If the intermediate transforms in stages (ii) and (iv) are performed *in place*, i.e. with the results overwriting the data, then at stage (v) the result $X^*(k_2^* + k_1^*N_2)$ will be found at address $k_1^* + N_1k_2^*$. This phenomenon is called *scrambling* by ‘digit reversal’, and stage (v) is accordingly known as *unscrambling*.

The initial N -point transform $\bar{F}(N)$ has thus been performed as N_1 transforms $\bar{F}(N_2)$ on N_2 points, followed by N_2 transforms $\bar{F}(N_1)$ on N_1 points, thereby reducing the arithmetic cost from $(N_1N_2)^2$ to $N_1N_2(N_1 + N_2)$. The phase shifts applied at stage (iii) are traditionally called ‘twiddle factors’, and the transposition between k_1 and k_2^* can be performed by the fast recursive technique of Eklundh (1972). Clearly, this procedure can be applied recursively if N_1 and N_2 are themselves composite, leading to an overall arithmetic cost of order $N \log N$ if N has no large prime factors.

The Cooley–Tukey factorization may also be derived from a geometric rather than arithmetic argument. The decomposition $k = k_1 + N_1k_2$ is associated to a geometric partition of the residual lattice $\mathbb{Z}/N\mathbb{Z}$ into N_1 copies of $\mathbb{Z}/N_2\mathbb{Z}$, each translated by $k_1 \in \mathbb{Z}/N_1\mathbb{Z}$ and ‘blown up’ by a factor N_1 . This partition in turn induces a (direct sum) decomposition of \mathbf{X} as

$$\mathbf{X} = \sum_{k_1} \mathbf{X}_{k_1},$$

where

$$\begin{aligned} X_{k_1}(k) &= X(k) \quad \text{if } k \equiv k_1 \pmod{N_1}, \\ &= 0 \quad \text{otherwise.} \end{aligned}$$

According to (i), \mathbf{X}_{k_1} is related to \mathbf{Y}_{k_1} by *decimation by N_1 and offset by k_1* . By Section 1.3.2.7.2, $\bar{F}(N)[\mathbf{X}_{k_1}]$ is related to $\bar{F}(N_2)[\mathbf{Y}_{k_1}]$ by *periodization by N_2 and phase shift by $e(k^*k_1/N)$* , so that

$$X^*(k^*) = \sum_{k_1} e\left(\frac{k^*k_1}{N}\right) Y_{k_1}^*(k_2^*),$$

the periodization by N_2 being reflected by the fact that $Y_{k_1}^*$ does not depend on k_1^* . Writing $k^* = k_2^* + k_1^*N_2$ and expanding k^*k_1 shows that the phase shift contains both the twiddle factor $e(k_2^*k_1/N)$ and the kernel $e(k_1^*k_1/N_1)$ of $\bar{F}(N_1)$. The Cooley–Tukey algorithm is thus naturally associated to the coset decomposition of a lattice modulo a sublattice (Section 1.3.2.7.2).

It is readily seen that essentially the same factorization can be obtained for $F(N)$, up to the complex conjugation of the twiddle factors. The normalizing constant $1/N$ arises from the normalizing constants $1/N_1$ and $1/N_2$ in $F(N_1)$ and $F(N_2)$, respectively.

Factors of 2 are particularly simple to deal with and give rise to a characteristic computational structure called a ‘butterfly loop’. If $N = 2M$, then two options exist:

(a) using $N_1 = 2$ and $N_2 = M$ leads to collecting the even-numbered coordinates of \mathbf{X} into \mathbf{Y}_0 and the odd-numbered coordinates into \mathbf{Y}_1

$$\begin{aligned} Y_0(k_2) &= X(2k_2), & k_2 &= 0, \dots, M-1, \\ Y_1(k_2) &= X(2k_2+1), & k_2 &= 0, \dots, M-1, \end{aligned}$$

and writing:

$$\begin{aligned} X^*(k_2^*) &= Y_0^*(k_2^*) + e(k_2^*/N)Y_1^*(k_2^*), \\ & \quad k_2^* = 0, \dots, M-1; \\ X^*(k_2^* + M) &= Y_0^*(k_2^*) - e(k_2^*/N)Y_1^*(k_2^*), \\ & \quad k_2^* = 0, \dots, M-1. \end{aligned}$$

This is the original version of Cooley & Tukey, and the process of formation of \mathbf{Y}_0 and \mathbf{Y}_1 is referred to as ‘decimation in time’ (i.e. decimation along the *data index \mathbf{k}*).

(b) using $N_1 = M$ and $N_2 = 2$ leads to forming

$$\begin{aligned} Z_0(k_1) &= X(k_1) + X(k_1 + M), & k_1 &= 0, \dots, M-1, \\ Z_1(k_1) &= [X(k_1) - X(k_1 + M)]e\left(\frac{k_1}{N}\right), & k_1 &= 0, \dots, M-1, \end{aligned}$$

then obtaining separately the even-numbered and odd-numbered components of \mathbf{X}^* by transforming \mathbf{Z}_0 and \mathbf{Z}_1 :

$$\begin{aligned} X^*(2k_1^*) &= Z_0^*(k_1^*), & k_1^* &= 0, \dots, M-1; \\ X^*(2k_1^* + 1) &= Z_1^*(k_1^*), & k_1^* &= 0, \dots, M-1. \end{aligned}$$

This version is due to Sande (Gentleman & Sande, 1966), and the process of separately obtaining even-numbered and odd-numbered results has led to its being referred to as ‘decimation in frequency’ (i.e. decimation along the *result index k^**).

By repeated factoring of the number N of sample points, the calculation of $F(N)$ and $\bar{F}(N)$ can be reduced to a succession of stages, the smallest of which operate on single prime factors of N . The reader is referred to Gentleman & Sande (1966) for a particularly lucid analysis of the programming considerations which help implement this factorization efficiently; see also Singleton (1969). Powers of two are often grouped together into factors of 4 or 8, which are advantageous in that they require fewer complex multiplications than the repeated use of factors of 2. In this approach, large prime factors P are detrimental, since they require a full P^2 -size computation according to the defining formula.

1.3.3.2.2. The Good (or prime factor) algorithm

1.3.3.2.2.1. Ring structure on $\mathbb{Z}/N\mathbb{Z}$

The set $\mathbb{Z}/N\mathbb{Z}$ of congruence classes of integers modulo an integer N [see e.g. Apostol (1976), Chapter 5] inherits from \mathbb{Z} not only the additive structure used in deriving the Cooley–Tukey factorization, but also a *multiplicative* structure in which the product of two congruence classes mod N is uniquely defined as the class of the ordinary product (in \mathbb{Z}) of representatives of each class. The multiplication can be distributed over addition in the usual way, endowing $\mathbb{Z}/N\mathbb{Z}$ with the structure of a *commutative ring*.

If N is composite, the ring $\mathbb{Z}/N\mathbb{Z}$ has *zero divisors*. For example, let $N = N_1N_2$, let $n_1 \equiv N_1 \pmod{N}$, and let $n_2 \equiv N_2 \pmod{N}$: then $n_1n_2 \equiv 0 \pmod{N}$. In the general case, a product of non-zero elements will be zero whenever these elements collect together all the factors of N . These circumstances give rise to a fundamental theorem in the theory of commutative rings, the *Chinese Remainder Theorem* (CRT), which will now be stated and proved [see Apostol (1976), Chapter 5; Schroeder (1986), Chapter 16].

1.3.3.2.2.2. The Chinese remainder theorem

Let $N = N_1N_2 \dots N_d$ be factored into a product of pairwise coprime integers, so that $\text{g.c.d.}(N_i, N_j) = 1$ for $i \neq j$. Then the system of congruence equations

$$\ell \equiv \ell_j \pmod{N_j}, \quad j = 1, \dots, d,$$

has a unique solution $\ell \pmod{N}$. In other words, each $\ell \in \mathbb{Z}/N\mathbb{Z}$ is