

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

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associated in a one-to-one fashion to the d -tuple $(\ell_1, \ell_2, \dots, \ell_d)$ of its residue classes in $\mathbb{Z}/N_1\mathbb{Z}, \mathbb{Z}/N_2\mathbb{Z}, \dots, \mathbb{Z}/N_d\mathbb{Z}$.

The proof of the CRT goes as follows. Let

$$Q_j = \frac{N}{N_j} = \prod_{i \neq j} N_i.$$

Since g.c.d. $(N_j, Q_j) = 1$ there exist integers n_j and q_j such that

$$n_j N_j + q_j Q_j = 1, \quad j = 1, \dots, d,$$

then the integer

$$\ell = \sum_{i=1}^d \ell_i q_i Q_i \pmod{N}$$

is the solution. Indeed,

$$\ell \equiv \ell_j q_j Q_j \pmod{N_j}$$

because all terms with $i \neq j$ contain N_j as a factor; and

$$q_j Q_j \equiv 1 \pmod{N_j}$$

by the defining relation for q_j .

It may be noted that

$$\begin{aligned} (q_i Q_i)(q_j Q_j) &\equiv 0 \pmod{N} \text{ for } i \neq j, \\ (q_j Q_j)^2 &\equiv q_j Q_j \pmod{N}, \quad j = 1, \dots, d, \end{aligned}$$

so that the $q_j Q_j$ are mutually orthogonal *idempotents* in the ring $\mathbb{Z}/N\mathbb{Z}$, with properties formally similar to those of mutually orthogonal *projectors onto subspaces* in linear algebra. The analogy is exact, since by virtue of the CRT the ring $\mathbb{Z}/N\mathbb{Z}$ may be considered as the direct product

$$\mathbb{Z}/N_1\mathbb{Z} \times \mathbb{Z}/N_2\mathbb{Z} \times \dots \times \mathbb{Z}/N_d\mathbb{Z}$$

via the two mutually inverse mappings:

- (i) $\ell \mapsto (\ell_1, \ell_2, \dots, \ell_d)$ by $\ell \equiv \ell_j \pmod{N_j}$ for each j ;
- (ii) $(\ell_1, \ell_2, \dots, \ell_d) \mapsto \ell$ by $\ell = \sum_{i=1}^d \ell_i q_i Q_i \pmod{N}$.

The mapping defined by (ii) is sometimes called the ‘CRT reconstruction’ of ℓ from the ℓ_j .

These two mappings have the property of sending sums to sums and products to products, i.e.:

- (i) $\ell + \ell' \mapsto (\ell_1 + \ell'_1, \ell_2 + \ell'_2, \dots, \ell_d + \ell'_d)$
 $\ell \ell' \mapsto (\ell_1 \ell'_1, \ell_2 \ell'_2, \dots, \ell_d \ell'_d)$
- (ii) $(\ell_1 + \ell'_1, \ell_2 + \ell'_2, \dots, \ell_d + \ell'_d) \mapsto \ell + \ell'$
 $(\ell_1 \ell'_1, \ell_2 \ell'_2, \dots, \ell_d \ell'_d) \mapsto \ell \ell'$

(the last proof requires using the properties of the idempotents $q_j Q_j$). This may be described formally by stating that the CRT establishes a *ring isomorphism*:

$$\mathbb{Z}/N\mathbb{Z} \cong (\mathbb{Z}/N_1\mathbb{Z}) \times \dots \times (\mathbb{Z}/N_d\mathbb{Z}).$$

1.3.3.2.2.3. The prime factor algorithm

The CRT will now be used to factor the N -point DFT into a tensor product of d transforms, the j th of length N_j .

Let the indices k and k^* be subjected to the following mappings:

- (i) $k \mapsto (k_1, k_2, \dots, k_d), k_j \in \mathbb{Z}/N_j\mathbb{Z}$, by $k_j \equiv k \pmod{N_j}$ for each j , with reconstruction formula

$$k = \sum_{i=1}^d k_i q_i Q_i \pmod{N};$$

- (ii) $k^* \mapsto (k_1^*, k_2^*, \dots, k_d^*), k_j^* \in \mathbb{Z}/N_j\mathbb{Z}$, by $k_j^* \equiv q_j k^* \pmod{N_j}$ for each j , with reconstruction formula

$$k^* = \sum_{i=1}^d k_i^* Q_i \pmod{N}.$$

Then

$$\begin{aligned} k^* k &= \left(\sum_{i=1}^d k_i^* Q_i \right) \left(\sum_{j=1}^d k_j q_j Q_j \right) \pmod{N} \\ &= \sum_{i,j=1}^d k_i^* k_j q_i q_j Q_i Q_j \pmod{N}. \end{aligned}$$

Cross terms with $i \neq j$ vanish since they contain all the factors of N , hence

$$\begin{aligned} k^* k &= \sum_{j=1}^d q_j Q_j^2 k_j^* k_j \pmod{N} \\ &= \sum_{j=1}^d (1 - n_j N_j) Q_j k_j^* k_j \pmod{N}. \end{aligned}$$

Dividing by N , which may be written as $N_j Q_j$ for each j , yields

$$\begin{aligned} \frac{k^* k}{N} &= \sum_{j=1}^d (1 - n_j N_j) \frac{Q_j}{N_j Q_j} k_j^* k_j \pmod{1} \\ &= \sum_{j=1}^d \left(\frac{1}{N_j} - n_j \right) k_j^* k_j \pmod{1}, \end{aligned}$$

and hence

$$\frac{k^* k}{N} \equiv \sum_{j=1}^d \frac{k_j^* k_j}{N_j} \pmod{1}.$$

Therefore, by the multiplicative property of $e(\cdot)$,

$$e\left(\frac{k^* k}{N}\right) \equiv \bigotimes_{j=1}^d e\left(\frac{k_j^* k_j}{N_j}\right).$$

Let $\mathbf{X} \in L(\mathbb{Z}/N\mathbb{Z})$ be described by a one-dimensional array $X(k)$ indexed by k . The index mapping (i) turns \mathbf{X} into an element of $L(\mathbb{Z}/N_1\mathbb{Z} \times \dots \times \mathbb{Z}/N_d\mathbb{Z})$ described by a d -dimensional array $X(k_1, \dots, k_d)$; the latter may be transformed by $\bar{F}(N_1) \otimes \dots \otimes \bar{F}(N_d)$ into a new array $X^*(k_1^*, k_2^*, \dots, k_d^*)$. Finally, the one-dimensional array of results $X^*(k^*)$ will be obtained by reconstructing k^* according to (ii).

The prime factor algorithm, like the Cooley–Tukey algorithm, reindexes a 1D transform to turn it into d separate transforms, but the use of coprime factors and CRT index mapping leads to the further gain that *no twiddle factors* need to be applied between the successive transforms (see Good, 1971). This makes up for the cost of the added complexity of the CRT index mapping.

The natural factorization of N for the prime factor algorithm is thus its factorization into prime powers: $\bar{F}(N)$ is then the tensor product of separate transforms (one for each prime power factor $N_j = p_j^{v_j}$) whose results can be reassembled without twiddle factors. The separate factors p_j within each N_j must then be dealt with by another algorithm (e.g. Cooley–Tukey, which does require twiddle factors). Thus, the DFT on a prime number of points remains undecomposable.

1.3.3.2.3. The Rader algorithm

The previous two algorithms essentially reduce the calculation of the DFT on N points for N composite to the calculation of smaller DFTs on prime numbers of points, the latter remaining irreducible. However, Rader (1968) showed that the p -point DFT for p an odd