

1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

prime can itself be factored by invoking some extra arithmetic structure present in $\mathbb{Z}/p\mathbb{Z}$.

1.3.3.2.3.1. *N an odd prime*

The ring $\mathbb{Z}/p\mathbb{Z} = \{0, 1, 2, \dots, p-1\}$ has the property that its $p-1$ non-zero elements, called *units*, form a *multiplicative group* $U(p)$. In particular, all units $r \in U(p)$ have a unique multiplicative inverse in $\mathbb{Z}/p\mathbb{Z}$, i.e. a unit $s \in U(p)$ such that $rs \equiv 1 \pmod{p}$. This endows $\mathbb{Z}/p\mathbb{Z}$ with the structure of a *finite field*.

Furthermore, $U(p)$ is a *cyclic group*, i.e. consists of the successive powers $g^m \pmod{p}$ of a generator g called a *primitive root mod p* (such a g may not be unique, but it always exists). For instance, for $p = 7$, $U(7) = \{1, 2, 3, 4, 5, 6\}$ is generated by $g = 3$, whose successive powers mod 7 are:

$$g^0 = 1, \quad g^1 = 3, \quad g^2 = 2, \quad g^3 = 6, \quad g^4 = 4, \quad g^5 = 5$$

[see Apostol (1976), Chapter 10].

The basis of Rader's algorithm is to bring to light a hidden regularity in the matrix $F(p)$ by permuting the basis vectors \mathbf{u}_k and \mathbf{v}_{k^*} of $L(\mathbb{Z}/p\mathbb{Z})$ as follows:

$$\begin{aligned} \mathbf{u}'_0 &= \mathbf{u}_0 \\ \mathbf{u}'_m &= \mathbf{u}_k \quad \text{with } k = g^m, \quad m = 1, \dots, p-1; \\ \mathbf{v}'_0 &= \mathbf{v}_0 \\ \mathbf{v}'_{m^*} &= \mathbf{v}_{k^*} \quad \text{with } k^* = g^{m^*}, \quad m^* = 1, \dots, p-1; \end{aligned}$$

where g is a primitive root mod p .

With respect to these new bases, the matrix representing $\bar{F}(p)$ will have the following elements:

$$\begin{aligned} \text{element } (0, 0) &= 1 \\ \text{element } (0, m+1) &= 1 \quad \text{for all } m = 0, \dots, p-2, \\ \text{element } (m^*+1, 0) &= 1 \quad \text{for all } m^* = 0, \dots, p-2, \\ \text{element } (m^*+1, m+1) &= e\left(\frac{k^*k}{p}\right) \\ &= e(g^{(m^*+m)/p}) \\ &\quad \text{for all } m^* = 0, \dots, p-2. \end{aligned}$$

Thus the 'core' $\bar{C}(p)$ of matrix $\bar{F}(p)$, of size $(p-1) \times (p-1)$, formed by the elements with two non-zero indices, has a so-called *skew-circulant* structure because element (m^*, m) depends only on $m^* + m$. Simplification may now occur because multiplication by $\bar{C}(p)$ is closely related to a *cyclic convolution*. Introducing the notation $C(m) = e(g^{m/p})$ we may write the relation $\mathbf{Y}^* = \bar{F}(p)\mathbf{Y}$ in the permuted bases as

$$\begin{aligned} Y^*(0) &= \sum_k Y(k) \\ Y^*(m^*+1) &= Y(0) + \sum_{m=0}^{p-2} C(m^*+m)Y(m+1) \\ &= Y(0) + \sum_{m=0}^{p-2} C(m^*-m)Z(m) \\ &= Y(0) + (\mathbf{C} * \mathbf{Z})(m^*), \quad m^* = 0, \dots, p-2, \end{aligned}$$

where \mathbf{Z} is defined by $Z(m) = Y(p-m-2)$, $m = 0, \dots, p-2$.

Thus \mathbf{Y}^* may be obtained by cyclic convolution of \mathbf{C} and \mathbf{Z} , which may for instance be calculated by

$$\mathbf{C} * \mathbf{Z} = F(p-1)[\bar{F}(p-1)[\mathbf{C}] \times \bar{F}(p-1)[\mathbf{Z}]],$$

where \times denotes the component-wise multiplication of vectors. Since p is odd, $p-1$ is always divisible by 2 and may even be

highly composite. In that case, factoring $\bar{F}(p-1)$ by means of the Cooley–Tukey or Good methods leads to an algorithm of complexity $p \log p$ rather than p^2 for $\bar{F}(p)$. An added bonus is that, because $g^{(p-1)/2} = -1$, the elements of $\bar{F}(p-1)[\mathbf{C}]$ can be shown to be either purely real or purely imaginary, which halves the number of real multiplications involved.

1.3.3.2.3.2. *N a power of an odd prime*

This idea was extended by Winograd (1976, 1978) to the treatment of prime powers $N = p^\nu$, using the cyclic structure of the multiplicative group of units $U(p^\nu)$. The latter consists of all those elements of $\mathbb{Z}/p^\nu\mathbb{Z}$ which are not divisible by p , and thus has $q_\nu = p^{\nu-1}(p-1)$ elements. It is cyclic, and there exist primitive roots g modulo p^ν such that

$$U(p^\nu) = \{1, g, g^2, g^3, \dots, g^{q_\nu-1}\}.$$

The $p^{\nu-1}$ elements divisible by p , which are divisors of zero, have to be treated separately just as 0 had to be treated separately for $N = p$.

When $k^* \notin U(p^\nu)$, then $k^* = pk_1^*$ with $k_1^* \in \mathbb{Z}/p^{\nu-1}\mathbb{Z}$. The results $X^*(pk_1^*)$ are p -decimated, hence can be obtained via the $p^{\nu-1}$ -point DFT of the $p^{\nu-1}$ -periodized data \mathbf{Y} :

$$X^*(pk_1^*) = \bar{F}(p^{\nu-1})[\mathbf{Y}](k_1^*)$$

with

$$Y(k_1) = \sum_{k_2 \in \mathbb{Z}/p\mathbb{Z}} X(k_1 + p^{\nu-1}k_2).$$

When $k^* \in U(p^\nu)$, then we may write

$$X^*(k^*) = X_0^*(k^*) + X_1^*(k^*),$$

where \mathbf{X}_0^* contains the contributions from $k \notin U(p^\nu)$ and \mathbf{X}_1^* those from $k \in U(p^\nu)$. By a converse of the previous calculation, \mathbf{X}_0^* arises from p -decimated data \mathbf{Z} , hence is the $p^{\nu-1}$ -periodization of the $p^{\nu-1}$ -point DFT of these data:

$$X_0^*(p^{\nu-1}k_1^* + k_2^*) = \bar{F}(p^{\nu-1})[\mathbf{Z}](k_2^*)$$

with

$$Z(k_2) = X(pk_2), \quad k_2 \in \mathbb{Z}/p^{\nu-1}\mathbb{Z}$$

(the $p^{\nu-1}$ -periodicity follows implicitly from the fact that the transform on the right-hand side is independent of $k_1^* \in \mathbb{Z}/p\mathbb{Z}$).

Finally, the contribution X_1^* from all $k \in U(p^\nu)$ may be calculated by reindexing by the powers of a primitive root g modulo p^ν , i.e. by writing

$$X_1^*(g^{m^*}) = \sum_{m=0}^{q_\nu-1} X(g^m)e(g^{(m^*+m)/p^\nu})$$

then carrying out the multiplication by the skew-circulant matrix core as a convolution.

Thus the DFT of size p^ν may be reduced to two DFTs of size $p^{\nu-1}$ (dealing, respectively, with p -decimated results and p -decimated data) and a convolution of size $q_\nu = p^{\nu-1}(p-1)$. The latter may be 'diagonalized' into a multiplication by purely real or purely imaginary numbers (because $g^{(q_\nu/2)} = -1$) by two DFTs, whose factoring in turn leads to DFTs of size $p^{\nu-1}$ and $p-1$. This method, applied recursively, allows the complete decomposition of the DFT on p^ν points into arbitrarily small DFTs.

1.3.3.2.3.3. *N a power of 2*

When $N = 2^\nu$, the same method can be applied, except for a slight modification in the calculation of \mathbf{X}_1^* . There is no primitive root modulo 2^ν for $\nu > 2$: the group $U(2^\nu)$ is the direct product of two cyclic groups, the first (of order 2) generated by -1 , the second (of order $N/4$) generated by 3 or 5. One then uses a representation