1.3.3.3.3.3. The Johnson–Burrus family of algorithms

In order to explore systematically all possible algorithms for carrying out a given DFT computation, and to pick the one best suited to a given machine, attempts have been made to develop:

(i) a high-level notation of describing all the ingredients of a DFT computation, including data permutation and data flow;

(ii) a formal calculus capable of operating on these descriptions so as to represent all possible reorganizations of the computation;

(iii) an automatic procedure for evaluating the performance of a given algorithm on a specific architecture.

Task (i) can be accomplished by systematic use of a tensor product notation to represent the various stages into which the DFT can be factored (reindexing, small transforms on subsets of indices, twiddle factors, digit-reversal permutations).

Task (ii) may for instance use the Winograd **CBA** normal form for each small transform, then apply the rules governing the rearrangement of tensor product $\bigotimes$ and ordinary product $\times$ operations on matrices. The matching of these rearrangements to the architecture of a vector and/or parallel computer can be formalized algebraically [see *e.g.* Chapter 2 of Tolimieri *et al.* (1989)].

Task (iii) is a complex search which requires techniques such as dynamic programming (Bellman, 1958).

Johnson & Burrus (1983) have proposed and tested such a scheme to identify the optimal trade-offs between prime factor nesting and Winograd nesting of small Winograd transforms. In step (ii), they further decomposed the pre-addition matrix **A** and post-addition matrix **C** into several factors, so that the number of design options available becomes very large: the N-point DFT when N has four factors can be calculated in over 10^{12} distinct ways.

This large family of nested algorithms contains the prime factor algorithm and the Winograd algorithms as particular cases, but usually achieves greater efficiency than either by reducing the f.p. multiplication count while keeping the number of f.p. additions small.

There is little doubt that this systematic approach will be extended so as to incorporate all available methods of restructuring the DFT.

1.3.4. Crystallographic applications of Fourier transforms

1.3.4.1. Introduction

The central role of the Fourier transformation in X-ray crystallography is a consequence of the kinematic approximation used in the description of the scattering of X-rays by a distribution of electrons (Bragg, 1915; Duane, 1925; Havighurst, 1925*a*,*b*; Zachariasen, 1945; James, 1948*a*, Chapters 1 and 2; Lipson & Cochran, 1953, Chapter 1; Bragg, 1975).

Let $\rho(\mathbf{X})$ be the density of electrons in a sample of matter contained in a finite region V which is being illuminated by a parallel monochromatic X-ray beam with wavevector $\mathbf{K}_0$. Then the far-field amplitude scattered in a direction corresponding to wavevector $\mathbf{K} = \mathbf{K}_0 + \mathbf{H}$ is proportional to

$$\begin{aligned} F(\mathbf{H}) &= \int_V \rho(\mathbf{X}) \exp(2\pi i \mathbf{H}\cdot\mathbf{X})\, \mathrm{d}^3\mathbf{X} \\ &= \bar{\mathscr{F}}[\rho](\mathbf{H}) \\ &= \langle \rho_{\mathbf{x}}, \exp(2\pi i \mathbf{H}\cdot\mathbf{X})\rangle. \end{aligned}$$

In certain model calculations, the 'sample' may contain not only volume charges, but also point, line and surface charges. These singularities may be accommodated by letting ρ be a distribution, and writing

$$F(\mathbf{H}) = \bar{\mathscr{F}}[\rho](\mathbf{H}) = \langle \rho_{\mathbf{x}}, \exp(2\pi i \mathbf{H}\cdot\mathbf{X})\rangle.$$

F is still a well behaved function (analytic, by Section 1.3.2.4.2.10) because ρ has been assumed to have compact support.

If the sample is assumed to be an infinite crystal, so that ρ is now a *periodic* distribution, the customary limiting process by which it is shown that F becomes a discrete series of peaks at reciprocal-lattice points (see *e.g.* von Laue, 1936; Ewald, 1940; James, 1948*a* p. 9; Lipson & Taylor, 1958, pp. 14–27; Ewald, 1962, pp. 82–101; Warren, 1969, pp. 27–30) is already subsumed under the treatment of Section 1.3.2.6.

1.3.4.2. Crystallographic Fourier transform theory

1.3.4.2.1. Crystal periodicity

1.3.4.2.1.1. Period lattice, reciprocal lattice and structure factors

Let ρ be the distribution of electrons in a crystal. Then, by definition of a crystal, ρ is Λ-*periodic* for some period lattice Λ (Section 1.3.2.6.5) so that there exists a motif distribution ρ^0 with compact support such that

$$\rho = R * \rho^0,$$

where $R = \sum_{\mathbf{x}\in\Lambda} \delta_{(\mathbf{X})}$. The lattice Λ is usually taken to be the finest for which the above representation holds.

Let Λ have a basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ over the integers, these basis vectors being expressed in terms of a standard orthonormal basis $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ as

$$\mathbf{a}_k = \sum_{j=1}^{3} a_{jk}\mathbf{e}_j.$$

Then the matrix

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

is the period matrix of Λ (Section 1.3.2.6.5) with respect to the unit lattice with basis $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, and the volume V of the unit cell is given by $V = |\det \mathbf{A}|$.

By Fourier transformation

$$\bar{\mathscr{F}}[\rho] = R^* \times \bar{\mathscr{F}}[\rho^0],$$

where $R^* = \sum_{\mathbf{H}\in\Lambda^*} \delta_{(\mathbf{H})}$ is the lattice distribution associated to the reciprocal lattice Λ^*. The basis vectors $(\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*)$ have coordinates in $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ given by the columns of $(\mathbf{A}^{-1})^T$, whose expression in terms of the cofactors of **A** (see Section 1.3.2.6.5) gives the familiar formulae involving the cross product of vectors for $n = 3$. The **H**-distribution F of scattered amplitudes may be written

$$F = \bar{\mathscr{F}}[\rho]_{\mathbf{H}} = \sum_{\mathbf{H}\in\Lambda^*} \bar{\mathscr{F}}[\rho^0](\mathbf{H})\delta_{(\mathbf{H})} = \sum_{\mathbf{H}\in\Lambda^*} F_{\mathbf{H}}\delta_{(\mathbf{H})}$$

and is thus a weighted reciprocal-lattice distribution, the weight $F_{\mathbf{H}}$ attached to each node $\mathbf{H} \in \Lambda^*$ being the value at **H** of the transform $\bar{\mathscr{F}}[\rho^0]$ of the motif ρ^0. Taken in conjunction with the assumption that the scattering is elastic, *i.e.* that **H** only changes the direction but not the magnitude of the incident wavevector $\mathbf{K}_0$, this result yields the usual forms (Laue or Bragg) of the