Discrete Fourier transform

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1. Introduction

The evaluation of the tree diagrams in instantaneous stochastic perturbation theory [1] requires the relevant free-field equations to be solved a large number of times. These calculations can be performed efficiently using the fast Fourier transform (see ref. [2], for example). Depending on the chosen boundary conditions for the fields, different forms of the Fourier transform need to be considered. In this note, a wide class of discrete Fourier transformations is introduced and their evaluation using the fast Fourier transform is described in some detail.

2. Transformation of periodic functions

In field theory, it is helpful to interpret the Fourier transform as a mapping of function spaces. The boundary conditions considered may then be encoded in the definition of the latter.

2.1 The function spaces $\mathcal{H}_n^b$

Let n be a natural number and $b \in \{0,1\}$ a one-bit integer. The space $\mathcal{H}_n^b$ consists of all complex functions $f(x)$, $x \in \mathbb{Z}$, satisfying

$$f(x+n) = (-1)^b f(x). \tag{2.1}$$

Since such functions are completely specified through eq. (2.1) and their values in the range $0 \leq x < n$, the dimension of $\mathcal{H}_n^b$ is equal to n. The scalar product of any two functions $f, g \in \mathcal{H}_n^b$ is defined by

$$(f, g) = \sum_{x=0}^{n-1} f(x)^* g(x), \tag{2.2}$$

where the star denotes complex conjugation.

2.2 Fourier transform

The Fourier transforms considered are maps

$$\mathcal{F}_n^{bc} : \mathcal{H}_n^b \mapsto \mathcal{H}_n^c \tag{2.3}$$

given by

$$\tilde{f}(k) = \sum_{x=0}^{n-1} \exp\Big\{ i \frac{2\pi}{n} \left(k + \tfrac{1}{2}b\right) \left(x + \tfrac{1}{2}c\right) \Big\} f(x) \tag{2.4}$$

for all functions $f \in \mathcal{H}_n^b$. In this expression, the shift $\frac{1}{2}c$ ensures that the Fourier transform $\tilde{f}$ is in $\mathcal{H}_n^c$, while the shift $\frac{1}{2}b$ turns the summand into a strictly periodic function of x. The summation range $[0, n)$ could thus be translated by any distance without changing the sum.

For all n, b, c, the inverse of the Fourier transform,

$$\left[\mathcal{F}_n^{bc}\right]^{-1} : \mathcal{H}_n^c \mapsto \mathcal{H}_n^b, \tag{2.5}$$

$$f(x) = \frac{1}{n} \sum_{k=0}^{n-1} \exp\Big\{ -i \frac{2\pi}{n} \left(x + \tfrac{1}{2}c\right) \left(k + \tfrac{1}{2}b\right) \Big\} \tilde{f}(k), \tag{2.6}$$

is of the same form apart from the prefactor $1/n$ and a change of sign in the argument of the exponential function. Fourier transforms are unitary with respect to the scalar product (2.2),

$$(\tilde{f}, \tilde{g}) = n(f, g), \tag{2.7}$$

up to a constant factor.

3. Dirichlet and Neumann boundary conditions

Dirichlet and Neumann boundary conditions can be conveniently imposed using the orbifold trick. There are different choices of the reflection points and a corresponding set of Fourier transforms.

3.1 The function spaces $\mathcal{K}_n^{bcd}$

Let n, b be as before and c, d further one-bit integers. The space $\mathcal{K}_n^{bcd}$ consists of all functions $f \in \mathcal{H}_{2n}^b$ that satisfy

$$f(-x-c) = (-1)^d f(x) \tag{3.1}$$

for all $x \in \mathbb{Z}$. These functions are completely specified by their values in the range $0 \leq x \leq n$, the reflection property (3.1) and the periodicity requirement (2.1) (with n replaced by $2n$).

Depending on b, c, d, the function values at $x = 0$ and $x = n$ are however constrained by the reflection and translation properties. The complete list of contraints is

$$f(n) = (-1)^{b+d} f(n-1) \quad \text{if} \quad c = 1, \tag{3.2}$$

and

$$f(0) = 0 \quad \text{if} \quad c = 0,\ d = 1, \tag{3.3}$$

$$f(n) = 0 \quad \text{if} \quad c = 0,\ b + d = 1. \tag{3.4}$$

The dimension of $\mathcal{K}_n^{bcd}$ is thus equal to n if $c = 1$ and otherwise equal to $n + 1$ (if $b = 0,\ d = 0$), n (if $b = 1$) or $n-1$ (if $b = 0,\ d = 1$). In the classical continuum limit, the boundary conditions satisfied by the functions in $\mathcal{K}_n^{bcd}$ are independent of c. The four possible combinations of b and d correspond to the possible combinations of Dirichlet and Neumann boundary conditions at $x = 0$ and $x = n$ (see table 1).

3.2 Fourier transform of functions in $\mathcal{K}_n^{bcd}$

Since $\mathcal{K}_n^{bcd} \subset \mathcal{H}_{2n}^b$, the Fourier operator $\mathcal{F}_{2n}^{bc}$ naturally acts on the functions $f \in \mathcal{K}_n^{bcd}$. A little algebra then shows that their Fourier transforms (2.4) are contained in $\mathcal{K}_n^{cbd}$. This is consistent with the fact that the dimensions of $\mathcal{K}_n^{bcd}$ and $\mathcal{K}_n^{cbd}$ are the same.

Table 1. Boundary conditions in the classical continuum limit

b	d	$x = 0$	$x = n$
0	0	N	N
0	1	D	D
1	0	N	D
1	1	D	N

The Fourier transform (2.4) can be rewritten in an alternative form where only the independent function values appear. In the case of the functions $f \in \mathcal{K}_n^{b1d}$, these expressions are

$$\tilde{f}(k) = \begin{cases} 2\sum_{x=0}^{n-1} \cos\Big\{\dfrac{\pi}{n}\left(k + \tfrac{1}{2}b\right)\left(x + \tfrac{1}{2}\right)\Big\} f(x) & \text{if } d = 0, \\ 2i\sum_{x=0}^{n-1} \sin\Big\{\dfrac{\pi}{n}\left(k + \tfrac{1}{2}b\right)\left(x + \tfrac{1}{2}\right)\Big\} f(x) & \text{if } d = 1, \end{cases} \tag{3.5}$$

while for the functions $f \in \mathcal{K}_n^{b0d}$ they are given by

$$\tilde{f}(k) = \begin{cases} 2{\sum_{x=0}^{n}}' \cos\Big\{\dfrac{\pi}{n}\left(k + \tfrac{1}{2}b\right) x\Big\} f(x) & \text{if } d = 0, \\ 2i{\sum_{x=0}^{n}}' \sin\Big\{\dfrac{\pi}{n}\left(k + \tfrac{1}{2}b\right) x\Big\} f(x) & \text{if } d = 1, \end{cases} \tag{3.6}$$

where the primed summation symbol indicates that the terminal summands are counted with weight 1/2.

Another useful observation concerns the inverse of the Fourier transform, which is related to the forward Fourier transform through

$$f(x) = \frac{(-1)^d}{2n}\left[\mathcal{F}_{2n}^{cb}\tilde{f}\right](x) \tag{3.7}$$

for all functions $f \in \mathcal{K}_n^{bcd}$.

4. Fast Fourier transform

In view of the fact that all Fourier transforms can be reduced to the application of the transformations (2.4) or (2.6), it suffices to consider the numerical evaluation of these. Moreover, since

$$\mathcal{F}_n^{bc} = \exp\Big\{i\frac{\pi}{2n}bc\Big\}\mathcal{R}_n^c\mathcal{F}_n^{00}\mathcal{R}_n^b, \tag{4.1}$$

$$\mathcal{R}_n^b : \mathcal{H}_n^e \mapsto \mathcal{H}_n^{e\wedge b}, \qquad \big[\mathcal{R}_n^b f\big](x) = \exp\Big\{i\frac{\pi}{n}bx\Big\}f(x), \tag{4.2}$$

attention can be restricted to the Fourier transform with shifts $b = c = 0$.

4.1 Recursion

If $n = 2m$ is even, the Fourier transform (2.4) may be rewritten in the form

$$\tilde{f}(k) = \tilde{f}^0(k) + \exp\Big\{i\frac{2\pi}{n}k\Big\}\tilde{f}^1(k), \tag{4.3}$$

$$\tilde{f}^b(k) = \sum_{x=0}^{m-1}\exp\Big\{i\frac{2\pi}{m}kx\Big\}f(2x+b). \tag{4.4}$$

The functions $\tilde{f}^0(k)$ and $\tilde{f}^1(k)$ coincide with the Fourier transforms of the function $f(x)$ restricted to the even and odd points x, respectively. Once these are computed for $k = 0, .., m-1$, the full function can be reconstructed through

$$\tilde{f}(k) = \tilde{f}^0(k) + \exp\Big\{i\frac{2\pi}{n}k\Big\}\tilde{f}^1(k), \tag{4.5}$$

$$\tilde{f}(k+m) = \tilde{f}^0(k) - \exp\Big\{i\frac{2\pi}{n}k\Big\}\tilde{f}^1(k). \tag{4.6}$$

The computation of the Fourier transform of a function in $\mathcal{H}_n^0$ has thus been reduced to the computation of the Fourier transform of two functions in $\mathcal{H}_m^0$.

Now if $n = 2^p m$ for some $p > 1$, the procedure can be repeated p times. At the end of the recursion, one is then left with the task of computing the Fourier transform of 2^p functions with m values. If m is fairly small, these Fourier transforms can be obtained directly (see appendix A). Once this is done, the calculated functions must be linearly combined according to eqs. (4.5),(4.6) until the Fourier transform of the input function is obtained.

4.2 Data reordering

The procedure outlined in the previous subsection requires a reordering of the function values $f(x)$ such that the 2^p functions that are to be transformed at the lowest level (those with m values) come one after another. The reordering

$$f(x) \to f(r(x)), \quad x = 0, \ldots, n-1, \tag{4.7}$$

is achieved with the help of an index array $r(x)$, which is constructed recursively.

Starting from the identity map, $r(x) = x$, the first step in the recursion moves the values $r(x)$ at the even positions x to the first $n/2$ positions in the array and the values at the odd positions to the remaining $n/2$ positions. The algorithm then visits the two blocks of $n/2$ positions one after the other and moves the array values within each block in the same way, i.e. such that those at the even positions come before those at the odd positions. At this point there are 4 blocks that get reordered one by one in the next step. The recursion ends after p steps when the blocks have size m.

4.3 Multi-dimensional Fourier transform

The Fourier transformation of a field $\phi(x)$ in more than one dimension can be performed in one direction after another. Each of these transformations may require the data to be rearranged in memory for efficient processing.

For the transformation in a direction with coordinate z, the field array should preferably be of the form `phi[z][i]`, where i is an index labeling the field elements at fixed z. The index may include the indices of the field (if any) but must not depend on z. With this data layout, the fast Fourier transform may be organized such that the innermost loop runs over the index i.

An MPI program can divide the loop over i among the processes in direction z. Locally missing data in the z direction must be fetched from the other processes and be returned to these after the Fourier transform is calculated. All this can be done so that each process has practically the same load.

Appendix A

For small n and $b = c = 0$, the Fourier transform (2.4) can be evaluated efficiently using trigonometric identities. For notational simplicity, $f(x)$ and $\tilde{f}(k)$ are written as f_x and $\tilde{f}_k$.

$n = 2$. In this case, the transformation

$$\tilde{f}_0 = f_0 + f_1, \tag{A.1}$$

$$\tilde{f}_1 = f_0 - f_1, \tag{A.2}$$

only requires additions and subtractions.

$n = 3$. Setting

$$u_1 = -\frac{1}{2}, \quad v_1 = \frac{\sqrt{3}}{2}, \tag{A.3}$$

the transformation is given by

$$z_1 = f_1 + f_2, \tag{A.4}$$

$$z_2 = v_1(f_1 - f_2), \tag{A.5}$$

$$z_3 = f_0 + u_1 z_1 \tag{A.6}$$

and

$$\tilde{f}_0 = f_0 + z_1, \tag{A.7}$$

$$\tilde{f}_1 = z_3 + iz_2, \tag{A.8}$$

$$\tilde{f}_2 = z_3 - iz_2. \tag{A.9}$$

$n = 4$. Setting

$$z_1 = f_0 + f_2, \tag{A.10}$$

$$z_2 = f_0 - f_2, \tag{A.11}$$

$$z_3 = f_1 + f_3, \tag{A.12}$$

$$z_4 = f_1 - f_3, \tag{A.13}$$

the transformation is given by

$$\tilde{f}_0 = z_1 + z_3 \tag{A.14}$$

$$\tilde{f}_1 = z_2 + iz_4, \tag{A.15}$$

$$\tilde{f}_2 = z_1 - z_3, \tag{A.16}$$

$$\tilde{f}_3 = z_2 - iz_4. \tag{A.17}$$

$n = 5$. Four constants,

$$u_2 = \frac{1}{1+\sqrt{5}}, \quad v_2 = \frac{\sqrt{5+\sqrt{5}}}{2\sqrt{2}}, \tag{A.18}$$

$$u_3 = -u_2 - \frac{1}{2}, \quad v_3 = 2u_2 v_2, \tag{A.19}$$

need to be introduced in this case. Setting

$$z_1 = f_1 + f_4, \tag{A.20}$$

$$z_2 = f_1 - f_4, \tag{A.21}$$

$$z_3 = f_2 + f_3, \tag{A.22}$$

$$z_4 = f_2 - f_3, \tag{A.23}$$

$$z_5 = v_3 z_4 + v_2 z_2, \tag{A.24}$$

$$z_6 = v_3 z_2 - v_2 z_4, \tag{A.25}$$

the Fourier transform is given by

$$\tilde{f}_0 = f_0 + z_1 + z_3, \tag{A.26}$$

$$w_1 = f_0 + u_2 z_1 + u_3 z_3, \tag{A.27}$$

$$w_2 = f_0 + u_3 z_1 + u_2 z_3, \tag{A.28}$$

$$\tilde{f}_4 = w_1 - iz_5, \tag{A.29}$$

$$\tilde{f}_3 = w_2 - iz_6, \tag{A.30}$$

$$\tilde{f}_1 = w_1 + iz_5, \tag{A.31}$$

$$\tilde{f}_2 = w_2 + iz_6. \tag{A.32}$$

In order to obtain the Fourier transform with opposite sign of the argument of the exponential function, it suffices to change the sign of the constants v_1, v_2, v_3 and of the terms proportional to i in eqs. (A.15),(A.17).

References

[1] M. Lüscher, *Instantaneous stochastic perturbation theory*, JHEP 1504 (2015) 142

[2] W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, *Numerical recipes in* `FORTRAN`*: the art of scientific computing*, 2nd ed. (Cambridge University Press, Cambridge, 1992)