On the physical relevance of the discrete Fourier transform

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We present a new form of the discrete Fourier transform, which has a clear physical meaning and can be used for interpolation purposes. The relation to the continuous Fourier transform and the Fourier series is pointed out. We also discuss the operations of smoothing and filtering on this form of the discrete Fourier transform.

Keywords: discrete Fourier transforms, interpolation

Introduction

This paper originated from the author's dissatisfaction with the way the discrete Fourier transform is usually presented in the literature. Although mathematically correct, the physical meaning of the common representation is unsatisfactory, and no direct relationship exists with the continuous Fourier transform and the Fourier series. We present the discrete Fourier transform in a form that is physically relevant and relates obviously to the continuous Fourier transformation and the Fourier series. We discuss some consequences of this form for the smoothing and filtering of the Fourier expansion. In a brief section on applications we discuss the usefulness of this discrete Fourier transform for interpolation purposes and its limitations, in particular the problem of aliasing. We also comment on the application of the fast Fourier transform (FFT) methods in the new context.

Basic Fourier theory

Let us first recall the standard Fourier theory for periodic functions. For a time function $x(t)$ with period T we can expand $x(t)$ as follows:

$$x(t) = a_0 + 2\sum_{n=1}^{\infty}\left\{a_n \cos\left(\frac{2\pi nt}{T}\right) + b_n \sin\left(\frac{2\pi nt}{T}\right)\right\} \quad (1)$$

where

$$a_n = \frac{1}{T}\int_0^T x(t)\cos\left(\frac{2\pi nt}{T}\right)dt \qquad n \geq 0$$
$$b_n = \frac{1}{T}\int_0^T x(t)\sin\left(\frac{2\pi nt}{T}\right)dt \qquad n \geq 1 \quad (2)$$

This so-called Fourier series is well known in the literature (e.g., Ref. 1, p. 204, and Ref. 2, p. 11). Also well known is the continuous Fourier transform (Ref. 1, p. 7, and Ref. 2, p. 11):

$$x(t) = \int_{-\infty}^{\infty} X(f)\exp(i2\pi ft)\,df \quad (3)$$

$$X(f) = \int_{-\infty}^{\infty} x(t)\exp(-i2\pi ft)\,dt \quad (4)$$

In statistics, engineering, and seismology one usually uses the coordinate t to indicate time (as in a time series), with the conjugate coordinate f representing the frequency and $2\pi f$ the angular frequency ω. In wave mechanics (Ref. 3, p. 118) one uses in addition to the conjugate pair (ω, t) the space ($\mathbf{r}$) and conjugate momentum coordinate ($\mathbf{k} = \mathbf{p}/\hbar$). In these latter cases, multiples of $(2\pi)^{1/2}$ appear in the transformation formulas (compare also the three different conventions listed by Bracewell[1] p. 7). In Fourier optics[4] one encounters yet another set of conjugate pairs, namely, the (x, y) coordinates of the observer and those of the object, with additional factors coming in for dimensional reasons.

In practice one does not observe a continuous time series but, for example, measures $x(t)$ at equidistant time intervals in a limited interval:

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$$t = r\Delta t \qquad r = 0,1,\ldots,N-1 \tag{5}$$

A similar situation can happen in Fourier optics when only a finite set of (equidistant) "observers" is present. In these cases the continuous Fourier transformation is replaced by the discrete Fourier transform (DFT), which is usually formulated as follows (Ref. 1, p. 358; Ref. 2, p. 12; Ref. 5, p. 100):

$$X_k = \frac{1}{N}\sum_{r=0}^{N-1} x_r \exp\left(-i\frac{2\pi kr}{N}\right) \qquad k = 0,1,\ldots,N-1 \tag{6}$$

The discrete time series can then be written in terms of the amplitudes X_k,

$$x_r = \sum_{k=0}^{N-1} X_k \exp\left(i\frac{2\pi kr}{N}\right) \qquad r = 0,1,\ldots,N-1 \tag{7}$$

where the "frequencies" are discretized according to

$$f_k = \frac{k}{N\Delta t} \qquad k = 0,1,\ldots,N-1 \tag{8}$$

While the mathematical symmetry of (6) and (7) is appealing, it is clear that (6)–(7) do not follow naturally from the set (3)–(4), since the frequencies in (6)–(7) run only over positive values, while the frequencies in (3) run equally over positive and negative values. Although equations (6)–(7) are mathematically correct, as can be easily proved using the identity

$$\sum_{k=0}^{N-1} \exp\left(-i\frac{2\pi kr}{N}\right) = \begin{cases} N & r = 0 \\ 0 & r = 1,2,\ldots,N-1 \end{cases} \tag{9}$$

they lack a clear physical meaning, as can be shown in various ways.

First, we note with Bracewell[1] (p. 360) that f_k cannot really be considered as a physical frequency. A time series $\{x_r\}$, with sampling period Δt, can be represented by a Fourier series consisting of a constant term plus multiples of the fundamental frequency $f_1 = 1/N\Delta t$. The highest frequency possible will be $\nu = 1/2\Delta t$, with two samples per period. However, f_k in (8) runs up to $\nu = (N-1)/N\Delta t \approx 1/\Delta t$; hence roughly half the frequencies in (8) are too high to be physically meaningful. The time series with interval time Δt should not be represented by functions that strongly oscillate between interval points.

A second way to demonstrate the physical inadequacy of (6)–(8) is to actually perform the summation in (7) and to see whether x_r behaves reasonably between the sample points r = integer, i.e., to see whether $x(r\Delta t)$ is a reasonable approximation to the original (continuous) time series $x(t)$. We can do the summation (7) for any real r and obtain

$$x(r\Delta t) = \frac{1}{N}\sum_{s=0}^{N-1} x_s \exp\left\{i\frac{N-1}{N}\pi(r-s)\right\} \times \frac{\sin\{\pi(r-s)\}}{\sin\{\pi(r-s)/N\}} \tag{10}$$

It is easy to check for integer r between 0 and $N-1$ that $x(r\Delta t) = x_r$, proving the mathematical correctness of (6)–(7). But if we want to determine $x(r\Delta t)$ midway between two integer values, we obtain

$$x\{(r+\tfrac{1}{2})\Delta t\} = \frac{1}{N}\sum_{s=0}^{N-1} x_s + \frac{i}{N}\sum_{s=0}^{N-1} x_s \cot\left\{\frac{\pi(r-s+\frac{1}{2})}{N}\right\} \tag{11}$$

As (11) shows, expression (7) is not a good approximation halfway between the sample points: first, the real part assumes the overall average $\bar{x}$ independent of the value of r; second, the imaginary part can be considerable, even if the original time series is real (note that the cotangent is proportional to N if $s \approx r$). This unphysical behavior is obviously due to the presence of the high frequencies in the series (7), so that, for example, the real part fluctuates wildly between the values x_r and $\bar{x}$.

The solution to these problems is to rewrite (7) into positive and negative frequencies as follows (take N is even first):

$$x_r = \sum_{k=0}^{N/2} X_k \exp\left(i\frac{2\pi kr}{N}\right)(1 - \tfrac{1}{2}\delta_{k,N/2}) + \sum_{k=N/2}^{N-1} X_k \exp\left(i\frac{2\pi kr}{N}\right)(1 - \tfrac{1}{2}\delta_{k,N/2}) \tag{12}$$

In the second sum we first replace k by $N - m$ and then replace X_{N-m} by X_{-m}, where we have extended the definition (6) for X_k to negative frequencies. We find

$$x_r = \sum_{k=0}^{N/2} X_k \exp\left(i\frac{2\pi kr}{N}\right)(1 - \tfrac{1}{2}\delta_{k,N/2}) + \sum_{m=1}^{N/2} X_{-m} \exp\left\{i\frac{2\pi(N-m)r}{N}\right\}(1 - \tfrac{1}{2}\delta_{m,N/2}) \tag{13}$$

Since r is an integer, we can drop the term $\exp(i2\pi r)$ and obtain after changing $m \to -k$ the following result:

$$x_r = \sum_{k=-N/2}^{N/2} X_k \exp\left(i\frac{2\pi kr}{N}\right)(1 - \tfrac{1}{2}\delta_{|k|,N/2}) \tag{14}$$

The odd case (N is odd) can be treated similarly, and we obtain the overall result

$$x_r = \sum_{k=-[N/2]}^{[N/2]} X_k \exp\left(i\frac{2\pi kr}{N}\right)(1 - \tfrac{1}{2}\delta_{|k|,N/2}) \qquad r = 0,1,\ldots,N-1 \tag{15}$$

where $[N/2] = (N-1)/2$ for odd N. Equation (15) has to be supplemented by the definition (6) for negative k,

$$X_k = \frac{1}{N}\sum_{r=0}^{N-1} x_r \exp\left(-i\frac{2\pi kr}{N}\right) \qquad k = 0, \pm 1, \ldots, \pm[N/2] \quad (16)$$

Since (15)–(16) were derived from (6)–(7), they are obviously correct mathematically. However, they also represent a natural extension of the continuous Fourier expansion (3)–(4) because of the symmetry in positive and negative frequencies. Nonetheless, I have not found a statement of (15)–(16) in the literature. An expression similar to (15) for even N is given by Bracewell[1] (p. 362). In his formulation the term $\frac{1}{2}X_{N/2}\exp(i\pi r)$ is combined with the term $\frac{1}{2}X_{-N/2}\exp(-i\pi r)$, using the fact that $X_{-N/2} = X_{N/2}$. This leads to the expression

$$x_r = \sum_{k=-N/2}^{N/2-1} X_k \exp\left(i\frac{2\pi kr}{N}\right) \quad (17)$$

However, this expression lacks the symmetry of (15), and if we allow r to become continuous in (17), we do not get the same physical acceptable results as in the case of (15)–(16), as we will see shortly.

In the case of (15)–(16) we get the following results for continuous r:

$$x(r\Delta t) = \frac{1}{N}\sum_{s=0}^{N-1} x_s \frac{\sin\{\pi(r-s)\}}{\sin\{\pi(r-s)/N\}} \qquad N = \text{odd} \quad (18)$$

and

$$x(r\Delta t) = \frac{1}{N}\sum_{s=0}^{N-1} x_s \frac{\sin\{\pi(r-s)\}}{\sin\{\pi(r-s)/N\}}\cos\{\pi(r-s)/N\} \qquad N = \text{even} \quad (19)$$

Obviously, $x(r\Delta t)$ now stays real, if the original time series x_s is real. By comparison, Bracewell's suggestion, (17) leads to

$$x(r\Delta t) = \frac{1}{N}\sum_{s=0}^{N-1} x_s \exp\{-i\pi(r-s)/N\} \times \frac{\sin\{\pi(r-s)\}}{\sin\{\pi(r-s)/N\}} \quad (20)$$

Hence $x(r\Delta t)$ is not real between interval points, even if the original series was real. Although this violation is not as serious as in the original expression, (10), it is still not acceptable physically, and we must insist on the set (15)–(16) as the physically acceptable discrete Fourier transform.

Relation of DFT to Fourier series

We have demonstrated how our discrete Fourier transform (DFT), equations (15)–(16), resembles the continuous Fourier expansion (3)–(4). Now we also want to establish a relationship with the Fourier series, (1)–(2). We rewrite (15) as follows:

$$x_r = a_0 + 2\sum_{k=1}^{[N/2]}\left\{a_k\cos\left(\frac{2\pi kr}{N}\right) + b_k\sin\left(\frac{2\pi kr}{N}\right)\right\} \times \left(1 - \frac{1}{2}\delta_{k,N/2}\right) \quad (21)$$

where

$$a_k = \frac{1}{2}(X_k + X_{-k}) = \frac{1}{N}\sum_{s=0}^{N-1} x_s \cos\left(\frac{2\pi ks}{N}\right) \qquad k = 0, 1, \ldots, [N/2] \quad (22)$$

and

$$b_k = \frac{i}{2}(X_k - X_{-k}) = \frac{1}{N}\sum_{s=0}^{N-1} x_s \sin\left(\frac{2\pi ks}{N}\right) \qquad k = 1, \ldots, [(N-1)/2] \quad (23)$$

We thus see that there is an obvious relationship between the Fourier series (1)–(2) and the expression (21)–(23) derived from (15)–(16) if we identify t as $r\Delta t$ and T as $N\Delta t$. Only the coefficient $\frac{1}{2}$, which occurs for N is even if $k = N/2$, was not obvious if one starts from (1)–(2). For real time series we can simply set

$$a_k = \text{Re}\,[X_k] \qquad b_k = -\text{Im}\,[X_k] \qquad k = 0, 1, \ldots, [N/2] \quad (24)$$

as $X_{-k} = X_k^*$ for real x_r.

Smoothing and filtering

Often the time series $x(t)$ contains noise, which typically has a high frequency. We can eliminate these frequencies by cutting out these contributions in (15). To do this process on the original series (7), which contains frequencies above the Nyquist frequency ($k = N/2$), is clearly unphysical. Instead we have to apply this process equally to the positive and negative frequencies in the physical series (15):

$$x_r = \sum_{k=-M}^{M} X_k \exp\left(i\frac{2\pi kr}{N}\right) \quad (25)$$

where $M < [N/2]$. The effect on the interpolation formulas (18)–(19) is easy to establish:

$$x(r\Delta t) = \frac{1}{N}\sum_{s=0}^{N-1} x_s \frac{\sin\{\pi(r-s)(2M+1)/N\}}{\sin\{\pi(r-s)/N\}} \quad (26)$$

For r is integer the dominant term in (26) occurs for $s = r$, leading to $[(2M+1)/N]\,x_r$, i.e., x_r with a reduced coefficient of <1. In addition, other x_s values now contribute to x_r. Obviously, expression (26) is no longer exact for r integer. Since band-pass and other filters[2] are often displayed for positive frequencies only, we may prefer to use (21)–(23), which contain only positive values of k but feature both sine and cosine functions. It should be obvious that a positive frequency filter applied to the original expression (7) leads to incorrect results, since the original expression is unphysical and contains frequencies higher than the Nyquist frequency. That is why we have some serious difficulties with the literature on seismic data processing (Ref. 2, p. 21), where positive frequency filters seem to be applied directly to (7).

Applications

The representation of a (time) series x_r by the discrete Fourier transform (15) should mainly be seen as a means of displaying the frequency content of the original series. Now that we have derived the correct physical representation of this series ((15) instead of (7) or (17)), one might ask how useful this series is for interpolation purposes. We must then keep in mind that the DFT automatically satisfies the periodicity property,

$$x\{(r+N)\Delta t\} = x(r\Delta t) \tag{27}$$

so that the DFT does not just try to mimic the original time series but also fits (27). The value of the DFT therefore depends strongly on whether the original physical time series is also periodic in accordance with (27). For example, if we try to represent the function

$$x(t_r) = \sin\left(\frac{\pi r \Delta t}{N\Delta t}\right) \tag{28}$$

with $t_r = r\Delta t$ for $r = 0,1,\ldots,N-1$, then the original function (28) satisfies the periodicity condition,

$$x(t_r + N\Delta t) = -x(t_r) \tag{29}$$

while the DFT satisfies (27). The DFT, which in this case reads

$$x^{\mathrm{DFT}}(t_r) \approx \frac{2}{\pi} - \frac{4}{3\pi}\cos\left(\frac{2\pi r}{N}\right) - \frac{4}{15\pi}\cos\left(\frac{4\pi r}{N}\right) - \ldots \tag{30}$$

will thus give an accurate description only on the interval $t = [0, N\Delta t]$, while on the interval $[N\Delta t, 2N\Delta t]$ it will give the wrong sign but about the right magnitude.

We found already that the expressions for the DFT known in the literature give an unphysical description of the original time series midway between the sample points. In these midway points our expression (18) or (19) leads to the approximation (we just include contributions of the closest points)

$$x\{(r+\tfrac{1}{2})\Delta t\} \approx \frac{2}{\pi}(x_r + x_{r+1}) \tag{31}$$

This result looks a bit counterintuitive, since one would expect the average of the contributions x_r and x_{r+1}. However, we have to realize that the sample points are equidistant, so that the points at $r-1$ and $r+2$ also contribute and improve the estimate through (15), or consequently, (18)–(19). In particular, for the special case of $N = 2$ we do obtain

$$x\left(\frac{1}{2}\Delta t\right) = \frac{1}{2}(x_0 + x_1) \tag{32}$$

It is also fairly easy to show that for constant $x_s = \bar{x}$ we get $x(r\Delta t) = \bar{x}$ for N is even and odd.

Let us finally comment on the case where the frequency ν of the time series is higher than the Nyquist frequency $\nu_{\mathrm{Ny}} = 1/2\Delta t$. In this case we encounter the problem of aliasing, when the higher-frequency component ν is represented by a lower-frequency component ν' in the DFT:

$$\nu' = \nu_{\mathrm{Ny}} - (\nu - \nu_{\mathrm{Ny}}) \tag{33}$$

as is described extensively in the literature.[2] We conclude that the DFT is especially suitable for interpolation purposes if the time series is periodic, with a periodicity manifest in the given time series.

Conclusions

We have given a new representation of the discrete Fourier transform, which correctly represents the frequency content of the given time series. The resulting series is related in a natural way to the continuous Fourier transform and the Fourier series. It can be used for interpolation purposes, especially when the given time series is periodic, and the periodicity is manifest in the given time series. The given representation also allows the correct use of frequency filters, by applying such filters equally to positive and negative frequencies. Since the common formulation of the DFT is mathematically correct, our results do not affect the usual fast Fourier methods,[6] although they may modify the interpretation of the frequency amplitudes and the use of filters.

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