

# Fourier analysis

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## Abstract

These notes review the basic theory of Fourier analysis. The emphasis is on the content that are necessary for one to correctly interpret and use the output of FFT computer libraries (e.g. FFTW).

## 1 Introduction

These notes were written when I was developing numerical codes that need to use FFT libraries. Like all students majoring in physics, I learned the Fourier series and Fourier transform in calculus courses when I was a undergraduate student. To apply this important mathematical method in practice, one additional necessary step is to know the Discrete Fourier Transform (DFT) and its fast numerical implementation, i.e., Fast Fourier Transform algorithm (FFT). There are many online material discussing these topics and I read some of them. But finally I found that I need to derive all the relevant formulas step by step by myself to convince myself that I fully understand the DFT and its many variations, such as discrete sine transform and cosine transform, and I am correctly using the output of FFT libraries.

Although the Fast Fourier Transform algorithm (FFT) is among the top ten algorithms that have changed the world, we do not need to know the details about this algorithm itself, which is simply an efficient way of computing the summation involved in the DFT. What we need to know is how the DFT is defined (so that we know how it can be used) and how it is related to the output of the various subroutines in various FFT computer libraries (e.g. FFTW). This is the emphasis of these notes, which give step by step derivation of the definition of DFT and its variation, the discrete sine transform.

## 2 Fourier series

### 2.1 Fourier series in terms of trigonometric functions cosine and sine

If  $h(x)$  is a function of period  $2L$ , then it can be proved that  $h(x)$  can be expressed as the following series

$$h(x) = \sum_{n=0}^{\infty} a_n \cos\left(\frac{n\pi}{L}x\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi}{L}x\right), \quad (1)$$

which is called the Fourier series. It is not trivial to prove the above statement (what is needed in the proof is to prove that the set of functions  $\cos(n\pi x/L)$  and  $\sin(n\pi x/L)$  with  $n = 0, 1, \dots, \infty$  is a “complete set”). We will not concern us here with this proof and simply start working with the Fourier series in Eq. (1). At this point it is not clear yet what the coefficients  $a_n$  and  $b_n$  are. Taking product of Eq. (1) with  $\cos(j\pi x/L)$  and  $\sin(j\pi x/L)$ , respectively, and then integrating from  $-L$  to  $L$ , we obtain

$$a_0 = \frac{1}{2L} \int_{-L}^L h(x) dx, \quad (2)$$

and for  $j \geq 1$ ,

$$a_j = \frac{1}{L} \int_{-L}^L h(x) \cos\left(\frac{j\pi}{L}x\right) dx, \quad (3)$$

$$b_j = \frac{1}{L} \int_{-L}^L h(x) \sin\left(\frac{j\pi}{L}x\right) dx. \quad (4)$$

In order to make the coefficients  $a_n$  be uniformly expressed by Eq. (3), we modify the Fourier series to the following form

$$h(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi}{L}x\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi}{L}x\right). \quad (5)$$

Then it is obvious that the coefficients  $a_0$  can be evaluated by using Eq. (3). Note that  $h(x)$  can be a complex-valued function (the independent variable  $x$  is still a real number). In this case, the coefficients  $a_n$  and  $b_n$  are complex numbers.

## 2.2 Fourier series in terms of complex-valued basis functions $e^{in\pi x/L}$

The Fourier series can also be expressed in terms of the complex-valued basis functions  $e^{in\pi x/L}$ . Next, we derive this form of the Fourier series. Using Euler's formula

$$\cos\left(\frac{n\pi}{L}x\right) = \frac{e^{in\pi x/L} + e^{-in\pi x/L}}{2} \quad (6)$$

and

$$\sin\left(\frac{n\pi}{L}x\right) = \frac{e^{in\pi x/L} - e^{-in\pi x/L}}{2i} \quad (7)$$

in Eq. (5), we obtain

$$h(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \frac{e^{in\pi x/L} + e^{-in\pi x/L}}{2} + \sum_{n=1}^{\infty} b_n \frac{e^{in\pi x/L} - e^{-in\pi x/L}}{2i}, \quad (8)$$

which can be further written

$$h(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[ \left( \frac{a_n - ib_n}{2} \right) e^{in\pi x/L} + \left( \frac{a_n + ib_n}{2} \right) e^{-in\pi x/L} \right]. \quad (9)$$

Define

$$c_n = \frac{a_n - ib_n}{2}, \quad c_{-n} = \frac{a_n + ib_n}{2}, \quad (10)$$

where  $n = 0, 1, 2, \dots, n$ , and note  $b_0 = 0$ , then Eq. (9) is written

$$h(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/L}. \quad (11)$$

Furthermore, using the expression of  $a_n$  and  $b_n$ , we find that  $c_n$  and  $c_{-n}$  in Eq. (10) can be uniformly expressed as

$$c_n = \frac{1}{2L} \int_{-L}^L h(x) e^{-in\pi x/L} dx. \quad (12)$$

Equations (11) along with Eq. (12) gives a compact form of the Fourier series[1]. On the other hand, using Eq. (10), the coefficients  $a_n$  and  $b_n$  can be recovered from  $c_n$  by

$$a_n = c_n + c_{-n}, \quad (13)$$

$$b_n = i(c_n - c_{-n}). \quad (14)$$

Note that if  $h(x)$  is real, then the coefficients  $a_n$  and  $b_n$  are real while the coefficient  $c_n$  are complex-valued. In this case, Eqs. (13) and (14) imply that  $c_n$  and  $c_{-n}$  must be complex conjugates.

[In the above, we use the basis functions  $e^{in\pi x/L}$  to expand  $h(x)$ . If we choose the basis functions to be  $e^{-in\pi x/L}$ , then it is ready to verify that the Fourier series are written

$$h(x) = \sum_{n=-\infty}^{\infty} c_n e^{-in\pi x/L}, \quad (15)$$

with  $c_n$  given by

$$c_n = \frac{1}{2L} \int_{-L}^L h(x) e^{in\pi x/L} dx. \quad (16)$$

In this case, the coefficients  $a_n$  and  $b_n$  can be recovered from  $c_n$  by

$$a_n = c_n + c_{-n} \quad (17)$$

$$b_n = -i(c_n - c_{-n}) \quad (18)$$

In using the Fourier series, we should be aware of which basis functions are used.]

### 3 From discrete spectrum to continuous spectrum: Fourier series→Fourier transformation

The Fourier series discussed above is written

$$h(t) = \sum_{n=-\infty}^{\infty} c_n e^{in2\pi t/T}, \quad (19)$$

where  $h(t)$  is a function of period  $T$ , the coefficient  $c_n$  is given by

$$c_n = \frac{1}{T} \int_{-T/2}^{T/2} h(t) e^{-in2\pi t/T} dt. \quad (20)$$

The  $n$ th term of the Fourier series corresponds to a harmonic with frequency

$$f_n = \frac{n}{T}. \quad (21)$$

In terms of  $f_n$ , the coefficient in Eq. (20) is written

$$c_n = c(f_n) = \frac{1}{T} \int_{-T/2}^{T/2} h(t) e^{-i2\pi t f_n} dt \quad (22)$$

In terms of  $f_n$ , the Fourier series in Eq. (19) is written

$$\begin{aligned} h(t) &= \sum_{n=-\infty}^{\infty} c(f_n) e^{i2\pi t f_n} \\ &= T \sum_{n=-\infty}^{\infty} c(f_n) e^{i2\pi t f_n} \frac{1}{T} \end{aligned} \quad (23)$$

Note that  $c(f_n) e^{i2\pi t f_n}$  is the value of function  $c(f) e^{i2\pi t f}$  at  $f = f_n$ . Further note that the interval between  $f_n$  and  $f_{n+1}$  is  $1/T$ . Thus the above summation is the rectangular formula for numerically calculating the integration  $\int_{-\infty}^{\infty} c(f) e^{i2\pi t f} df$ . Therefore, Eq. (23) can be approximately written

$$h(t) \approx T \int_{-\infty}^{\infty} c(f) e^{i2\pi t f} df, \quad (24)$$

which will become exact when the interval  $1/T \rightarrow 0$ , i.e.,  $T \rightarrow \infty$ . Therefore, for the case  $T \rightarrow \infty$ , the Fourier series exactly becomes

$$h(t) = T \int_{-\infty}^{\infty} c(f) e^{i2\pi t f} df, \quad (25)$$

where  $c(f)$  is given by Eq. (22), i.e.,

$$c(f) = \frac{1}{T} \int_{-\infty}^{\infty} h(t) e^{-i2\pi t f} dt. \quad (26)$$

Note that the function  $h(t)$  given in Eqs. (25) is proportional to  $Tc(f)$  while the function  $c(f)$  given in Eq. (26) is proportional to  $1/T$ . Since  $T \rightarrow \infty$ , it is desired to eliminate the  $T$  and  $1/T$  factors in Eqs. (25) and (26), which can be easily achieved by defining a new function

$$H(f) = Tc(f). \quad (27)$$

Then the Fourier series is written

$$h(t) = \int_{-\infty}^{\infty} H(f) e^{i2\pi t f} df, \quad (28)$$

$$H(f) = \int_{-\infty}^{\infty} h(t) e^{-i2\pi t f} dt. \quad (29)$$

Equations (28) and (29) are the Fourier transformation pairs discussed in the next section. [Note that the signs in the exponential of Eq. (28) and (29) are opposite. Which one should be minus or positive is actually a matter of convention because a trivial variable substitution  $f' = -f$  can change the sign between minus and positive. Proof. In terms of  $f'$ , Eq. (28) is written

$$\begin{aligned} h(t) &= \int_{-\infty}^{\infty} H(-f') e^{-i2\pi t f'} d(-f'), \\ &= \int_{-\infty}^{\infty} H(-f') e^{-i2\pi t f'} df', \end{aligned} \quad (30)$$

Define

$$\begin{aligned} \bar{H}(f') &\equiv H(-f') \\ &= \int_{-\infty}^{\infty} h(t) e^{i2\pi t f'} dt. \end{aligned} \quad (31)$$

Then Eq. (30) is written

$$h(t) = \int_{-\infty}^{\infty} \bar{H}(f') e^{-i2\pi t f'} df' \quad (32)$$

The signs in the exponential of Eqs. (31) and (32) are opposite to Eqs. (29) and (28), respectively.]

In the following, I use (31) as the forward Fourier transformation and Eq. (32) as the backward one (this is the convention used in the book “Numerical recipe”[2]). However, it seems that the form in Eqs. (28) and (29) are often used in practice, i.e.,  $h(t)$  is expanded in terms of the basis function  $e^{i2\pi t f}$  instead of  $e^{-i2\pi t f}$ . The extensively used free software FFTW uses Eqs. (29) as the forward transformation and Eq. (28) as the backward one. When using a Fourier transformation library, it is necessary to know which convention is used in order to correctly use the output of the library.

## 4 Fourier transformation

As discussed above, the Fourier transformation of a function  $h(t)$  is given by

$$H(f) = \int_{-\infty}^{\infty} h(t) e^{i2\pi f t} dt. \quad (33)$$

Once the Fourier transformation  $H(f)$  is known, the original function  $h(t)$  can be reconstructed via

$$h(t) = \int_{-\infty}^{\infty} H(f) e^{-i2\pi f t} df. \quad (34)$$

[Physicists usually prefer to use the angular frequency  $\omega \equiv 2\pi f$  instead of the frequency  $f$  to represent the Fourier transformation. Using  $\omega$ , equations. (33) and (34) are written, respectively, as

$$H(\omega) = \int_{-\infty}^{\infty} h(t) e^{i\omega t} dt, \quad (35)$$

$$h(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} H(\omega) e^{-i\omega t} d\omega, \quad (36)$$

where we see that the asymmetry between the Fourier transformation and its inverse is more severe in this representation: besides the opposite-sign in the exponents, there is also a  $1/2\pi$  factor difference between the Fourier transformation and its inverse. Whether the  $1/2\pi$  factor appears at the forward transformation or inverse one is actually a matter of convention. The only requirement is that the product of the two factors in the forward and inverse transformation is equal to  $1/2\pi$ . To obtain a more symmetric pair, one can adopt a factor  $1/\sqrt{2\pi}$  at both the forward and inverse transformation. The representation in Eqs. (33) and (34) is adopted in this article. But we should know how to change to the  $\omega$  representation when needed.]

Next, consider how to numerically compute the Fourier transformation of a function  $h(t)$ . A simple way is to use the rectangle formula to approximate the integration in Eq. (33), i.e.,

$$H(f) \approx \Delta \sum_{j=-\infty}^{\infty} h_j \exp(i2\pi f j \Delta), \quad (37)$$

where  $h_j = h(t_j)$  and  $t_j = j\Delta$  with  $j = \dots, -2, -1, 0, 1, 2, \dots$ . Note Eq. (37) is an approximation, which will become exact if  $\Delta \rightarrow 0$ . In practice, we can sample  $h(t)$  only with a nonzero  $\Delta$ . Therefore Eq. (37) is usually an approximation. Do we have some rules to choose a suitable  $\Delta$  so that Eq. (37) can become a good approximation or even an exact relation? This important question is answered by the well-known sampling theorem, which states that a suitable  $\Delta$  to make Eq. (37) exact is given by  $\Delta \leq 1/(2f_c)$ , where  $f_c$  is the largest frequency contained in  $h(t)$  (i.e.,  $H(f) = 0$  for  $|f| > f_c$ ).

#### 4.1 Sampling theorem

In computational and experimental work, we know only a list of values  $h(t_j)$  sampled at discrete values of  $t_j$ . Let us suppose that  $h(t)$  is sampled with uniform interval between consecutive points:

$$h_j = h(t_j), t_j = j\Delta, j = \dots, -2, -1, 0, 1, 2, \dots \quad (38)$$

The sampling rate is defined by  $f_s = 1/\Delta$ . The sampling theorem states that: If the Fourier transformation of function  $h(t)$ ,  $H(f)$ , has the following property

$$H(f) = 0 \quad \text{for } |f| \geq f_c \quad (39)$$

then sampling  $h(t)$  with the sampling rate  $f_s \geq 2f_c$  (i.e.,  $\Delta \leq 1/(2f_c)$ ) will completely determine  $h(t)$ , which is given explicitly by the formula

$$h(t) = \Delta \sum_{j=-\infty}^{\infty} h_j \frac{\sin[2\pi f_c(t - j\Delta)]}{\pi(t - j\Delta)}. \quad (40)$$

We will not concern us here with the proof of the sampling theorem and simply start working with Eq. (40) to derive the concrete expression for the Fourier transformation of  $h(t)$ . Substituting the expression (40) for  $h(t)$  into the Fourier transformation (33), we obtain the explicit form of the Fourier transformation of  $h(t)$ :

$$\begin{aligned} H(f) &= \int_{-\infty}^{\infty} h(t) \exp(i2\pi f t) dt, \\ &= \Delta \sum_{j=-\infty}^{\infty} h_j \int_{-\infty}^{\infty} \frac{\sin[2\pi f_c(t - j\Delta)]}{\pi(t - j\Delta)} \exp(i2\pi f t) dt, \\ &= \Delta \sum_{j=-\infty}^{\infty} h_j \exp(i2\pi f j \Delta) \int_{-\infty}^{\infty} \frac{\sin[2\pi f_c(t - j\Delta)]}{\pi(t - j\Delta)} \exp[i2\pi f(t - j\Delta)] dt, \\ &= \Delta \sum_{j=-\infty}^{\infty} h_j \exp(i2\pi f j \Delta) \int_{-\infty}^{\infty} \frac{\sin[2\pi f_c \tau]}{\pi \tau} \exp[i2\pi f \tau] d\tau. \end{aligned} \quad (41)$$

With the help of Wolfram Mathematica, the integration in Eq. (41) is evaluated analytically, giving

$$\int_{-\infty}^{\infty} \frac{\sin[2\pi f_c \tau]}{\pi \tau} \exp(i2\pi f \tau) d\tau = \begin{cases} 0 & \text{For } |f| > f_c \\ 1 & \text{For } |f| < f_c \end{cases}. \quad (42)$$

Using this, Eq. (41) is written

$$H(f) = \begin{cases} 0 & \text{for } |f| > f_c \\ \Delta \sum_{j=-\infty}^{\infty} h_j \exp(i2\pi f j \Delta) & \text{for } |f| \leq f_c \end{cases}, \quad (43)$$

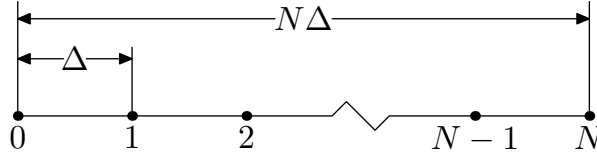
which shows that  $H(f) = 0$  for  $|f| > f_c$ , which is consistent with the assumption of sampling theorem, i.e.,  $H(f)$  has the property given in Eq. (39). The second line of Eq. (43) is identical to Eq. (37) except that Eq. (43) in this case is exact while Eq. (37) is only approximate. In other words, if  $\Delta \leq 1/(2f_c)$ , then the Fourier transformation is exactly given by Eq. (43), where  $f_c$  is the largest frequency contained in  $h(t)$  (i.e.,  $H(f) = 0$  for  $|f| > f_c$ ).

## 4.2 Discrete Fourier transformation

Suppose that a function  $h(t)$  is sampled with a sampling frequency  $f_s = 1/\Delta$ , and we know (by some other means) that the largest frequency contained in  $h(t)$  is less than  $f_s/2$ , then the sampling theorem indicates that the Fourier transformation  $H(f)$  for  $|f| \leq f_s/2$  can be written as

$$H(f) = \Delta \sum_{j=-\infty}^{\infty} h_j \exp(i2\pi f j \Delta). \quad (44)$$

Assume that the function  $h(t)$  is periodic with period  $T$  and is sampled in one period with  $h_j$  with  $j = 0, 1, \dots, N$ , in which  $h_0 = h_N$ , as shown in Fig. 1.



**Figure 1.** Sampling points in one period of the signal, where  $T = N\Delta$  is the period of the signal.

Then the infinite summation in Eq. (44) reduces to the following partial summation:

$$H(f) = C\Delta \sum_{j=0}^{N-1} h_j \exp(i2\pi f j \Delta), \quad (45)$$

where  $C$  is the number of periods during the infinite time. Note that, the partial summation in Eq. (45) includes  $N$  values of  $h(t)$  ( $h_N$  is excluded since it is identical to  $h_0$ ). With  $N$  inputs, we can expect at most  $N$  independent outputs. Further note that the frequency is limited in the range  $[-f_s/2, f_s/2]$  by the sampling theorem. Therefore, a simple way to select the  $N$  outputs from Eq. (45) is to evaluate  $H(f)$  at uniformly distributed frequencies  $f_n$  given by

$$f_n = f_s \frac{n}{N}, \quad (46)$$

with  $n = -\frac{N}{2}, \dots, -1, 0, 1, \dots, \frac{N}{2}$ . (we consider only the case that  $N$  is an even number; the above expression actually contains  $N + 1$  outputs). Evaluate Eq. (45) at  $f = f_n$ , then  $H(f_n)$  is written as

$$H(f_n) = C\Delta \sum_{j=0}^{N-1} h_j \exp\left(\frac{2\pi i}{N} n j\right). \quad (47)$$

The partial summation in Eq. (47),

$$H_n \equiv \sum_{j=0}^{N-1} h_j \exp\left(\frac{2\pi i}{N} n j\right), \quad (48)$$

is called the **Discrete Fourier transformation (DFT)**. Using Eqs. (47) and (48), we have

$$H(f_n) = C \Delta H_n. \quad (49)$$

### 4.3 Periodic property of Discrete Fourier transformation

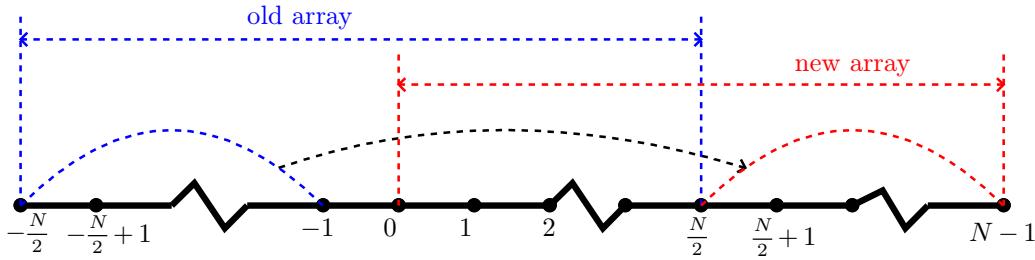
The DFT of time-domain array  $h_j$  with  $j = 0, 1, \dots, N - 1$  is given by Eq. (48), i.e.,

$$H_n = \sum_{j=0}^{N-1} W^{nj} h_j \quad (50)$$

with  $n = -N/2, \dots, N/2$ , where  $W = \exp\left(\frac{2\pi i}{N}\right)$ . Note that the subscript of  $H_n$  is in the range  $n = -N/2, \dots, N/2$  while the subscript of  $h_j$  is in the range  $j = 0, 1, \dots, N - 1$ . Further note that  $H_n$  contains  $N + 1$  elements while  $h_j$  contains only  $N$  elements. It is ready to find that the array defined in Eq. (50) has the following periodic property

$$H_{n+N} = H_n. \quad (51)$$

Using this general property, we obtain  $H_{-N/2} = H_{N/2}$ , i.e., the two ending elements of  $H_n$ , namely  $H_{-N/2}$  and  $H_{N/2}$ , are equal to each other. Thus only one value is needed to be stored. This can be used to reduce the number of elements of  $H_n$  needing to be stored by one. Then  $H_n$  contains only  $N$  elements, instead of  $N + 1$ . Furthermore, we prefer to make the index of  $H_n$  and  $h_j$  array have the same range, i.e., we prefer to make the index  $n$  of  $H_n$  array also in the range  $[0, N - 1]$ . This can be done by storing the negative frequency part (i.e.,  $n = -N/2, \dots, -1$ ) of  $H_n$  in the location where the subscripts are respectively  $n = N/2, \dots, N - 1$ , as is shown in Fig 2. A native method of implementing this in a code is to first calculate the values of  $H_n$  in the range  $n = -N/2, \dots, N/2$ , then shift the array to achieve the desired storage arrangement, as is shown in Fig 2. It turns out that we have a better way to achieve the same goal: using again the periodic property Eq. (51), we know that the value of the  $H_n$  array elements with negative subscripts,  $n = -N/2, \dots, -1$ , happens to be equal to the value of the  $H_n$  elements with subscripts  $n = N/2, \dots, N - 1$ , respectively. Using this, we can simply use Eq. (50) to calculate values of  $H_n$  in the range  $n = 0, 1, \dots, N - 1$  and the array obtained is exactly in the desired storage arrangement.



**Figure 2.** The negative frequency parts of the discrete Fourier transformation are stored at the locations with the array index  $n = \frac{N}{2}, \frac{N}{2} + 1, \dots, N - 1$ . Since  $H_{-N/2} = H_{N/2}$ , the location  $j = N/2$  of the new array can be considered to be storing both of them.

Of course, in practice, we do not use Eq. (50) directly to calculate  $H_n$ . Instead, the famous Fast Fourier Transformation (FFT) algorithm is used to calculate  $H_n$  with  $n = 0, 1, \dots, N - 1$ . Remember the storage arrangement discussed above is important for one to correctly interpret and use the output of FFT. For example, what frequency does the element  $H_j$  with  $j > N/2$  correspond to? The answer is obvious if we know the storage arrangement of FFT output: the corresponding frequency of No.  $j$ th element is given by

$$f_j = \begin{cases} \frac{j}{N} f_s, & \text{for } 0 \leq j \leq \frac{N}{2} \\ \frac{(j-N)}{N} f_s, & \text{for } \frac{N}{2} < j \leq N-1 \end{cases} \quad (52)$$

Therefore the frequency of  $H_j$  with  $j > N/2$  is  $(j - N)f_s/N$ . Define  $f_1 = 1/T$ , which is the fundamental frequency of the signal, then Eq. (52) can also be written as

$$f_j = \begin{cases} jf_1, & \text{for } 0 \leq j \leq \frac{N}{2} \\ (j - N)f_1, & \text{for } \frac{N}{2} < j \leq N - 1 \end{cases} \quad (53)$$

Q: What is the negative frequency counterpart of the element  $H_j$  for  $j \neq 0$ ? A: Examining the storage arrangement shown in Fig. 2, we know it is the element  $H_{N-j}$ .

#### 4.4 Aliasing errors

Signals that are not band-limited usually contains all frequencies and thus do not satisfy the condition that the sampling theorem requires (i.e.,  $H(f) = 0$  for  $|f| > 1/(2\Delta)$ ). In this case, for any given  $N$  data, we can still calculate its DFT by using Eq. (48). However the results obtained are meaningful only when  $H_n$  approaches zero as the frequency approaches  $-1/(2\Delta)$  from above and approaches  $1/(2\Delta)$  from below, i.e., only when the results obtained are consistent with the assumption used to obtain the results (the assumption is that  $H(f) = 0$  for  $|f| > 1/(2\Delta)$ ). When the results obtained do not satisfy the above condition, then it indicates that the “aliasing errors” have contributed to the results. We can reduce the aliasing errors by increasing the sampling frequency. The aliasing errors can be reduced but can not be completely removed for a non-band-limited signal. More details on the aliasing errors are needed here, to be continued.

#### 4.5 Relation between Fourier series coefficients and DFTs

In the above, we go through the process “Fourier series  $\rightarrow$  Fourier transformation  $\rightarrow$  DFT”. This corresponds to going from the discrete case (Fourier series) to the continuous case (Fourier transformation), and then back to the discrete case (DFT). Since both Fourier series and DFT are discrete, it is instructive to examine the relation between the Fourier coefficient  $c_n$  and the DFT  $H_n$ .

The Fourier coefficient is given by Eq. (20), i.e.,

$$c_n = \frac{1}{T} \int_{-T/2}^{T/2} h(t) e^{in2\pi t/T} dt, \quad (54)$$

which can be equivalently written

$$c(f_n) = \frac{1}{T} \int_{-T/2}^{T/2} h(t) e^{i2\pi t f_n} dt, \quad (55)$$

where  $f_n = n/T$ . If  $h(t)$  is sampled with sampling rate  $f_s = 1/\Delta$ , then the number of sampling points per period is  $N = T/\Delta$ . Then the frequency used to evaluate the DFT [Eq. (46)] is written

$$f_n = \frac{n}{\Delta N} = \frac{n}{T}, \quad (56)$$

which turns out to be identical to the frequency to which the Fourier coefficient  $c_n$  corresponds. Using  $f_n = n/(\Delta N)$  in Eq. (55), we obtain

$$\begin{aligned} c(f_n) &= \frac{1}{T} \int_{-T/2}^{T/2} h(t) \exp\left(\frac{i2\pi t n}{\Delta N}\right) dt. \\ &\approx \frac{1}{T} \Delta \sum_{j=0}^{N-1} h_j \exp\left(\frac{2\pi i}{N} n j\right) \end{aligned} \quad (57)$$

$$\begin{aligned} &= \frac{1}{T} \Delta H_n \\ &= \frac{1}{N} H_n \end{aligned} \quad (58)$$

i.e., the relation between the Fourier coefficient  $c_n$  and the DFT  $H_n$  is  $H_n = N c_n$ . Note that the approximation in Eq. (57) becomes an exact relation if the largest frequency contained in  $h(t)$  is less than  $1/(2\Delta)$ .



## 4.6 Reconstruct the original function using DFT

The Fourier series of  $h(t)$

$$h(t) = \sum_{n=-\infty}^{\infty} c_n e^{-in2\pi t/T} \quad (59)$$

can be approximated as

$$\begin{aligned} h(t) &\approx \sum_{n=-N/2}^{N/2} c_n e^{-in2\pi t/T} \\ &\approx \frac{1}{N} \sum_{n=-N/2}^{N/2} H_n e^{-in2\pi t/T} \end{aligned} \quad (60)$$

Using the periodic property of DFT, i.e.,  $H_n = H_{N+n}$ , the above expression is written as

$$h(t) = \frac{1}{N} \left[ \sum_{n=0}^{N/2} H_n e^{-in2\pi t/T} + \sum_{n=N/2}^{N-1} H_n e^{-i(n-N)2\pi t/T} \right]. \quad (61)$$

Equation (61) provide the formula of constructing an approximate function using the DFT of the discrete samplings of the original function.

## 4.7 Evaluate the reconstructed function at discrete points

Evaluate  $h(t)$  given by Eq. (61) at the discrete point  $t = j\Delta$ , yielding

$$\begin{aligned} h_j &\equiv h(j\Delta) = \frac{1}{N} \left[ \sum_{n=0}^{N/2} H_n e^{-in2\pi j/N} + \sum_{n=N/2}^{N-1} H_n e^{-i(n-N)2\pi j/N} \right] \\ &= \frac{1}{N} \left[ \sum_{n=0}^{N/2} H_n e^{-in2\pi j/N} + \sum_{n=N/2}^{N-1} H_n e^{-in2\pi j/N} \right] \\ &= \frac{1}{N} \left[ \sum_{n=0}^{N-1} H_n e^{-in2\pi j/N} + H_{N/2} e^{-i\pi j} \right] \\ &\approx \frac{1}{N} \sum_{n=0}^{N-1} H_n e^{-in2\pi j/N}. \end{aligned} \quad (62)$$

Equation (62) is actually the inverse DFT discussed in Sec. 4.8.

## 4.8 Inverse Discrete Fourier transformation

The DFT in Eq. (48),

$$H_n \equiv \sum_{j=0}^{N-1} h_j \exp\left(\frac{2\pi i}{N} nj\right),$$

with  $j = 0, 1, 2, \dots, N-1$  and  $n = 0, 1, 2, \dots, N-1$  can also be considered as a set of linear algebraic equations for  $h_j$  and can be solved in terms of  $H_n$ , which gives

$$h_j = \frac{1}{N} \sum_{n=0}^{N-1} H_n \exp\left(-\frac{2\pi i}{N} nj\right). \quad (63)$$

(The details on how to solve Eq. (48) to obtain the solution (63) is provided in Appendix 4.10.) Equation (63) recovers  $h_j$  from  $H_n$  (i.e., the DFT of  $h_j$ ), and thus is called the inverse DFT.

The normalization factor multiplying the DFT and inverse DFT (here 1 and  $1/N$ ) and the signs of the exponents are merely conventions, and differ in some treatments. The only requirements of these conventions are that the DFT and inverse DFT have opposite-sign exponents and that the product of their normalization factors be  $1/N$ .

## 4.9 About using the FFTW library

I use the Fortran interface of the FFTW library. To have access to FFTW library, use the following codes:

```
use, intrinsic :: iso_c_binding
implicit none
include 'fftw3.f03'
```

To use the FFT subroutines in FFTW, we need to define some variables of the desired types, such as

```
type(C_PTR) :: plan
complex(C_DOUBLE_COMPLEX) :: in(0:n-1), out(0:n-1)
```

Store input data in the “in” arrays, then, we can perform a DFT by the following codes:

```
plan = fftw_plan_dft_1d(n, in, out, FFTW_FORWARD, FFTW_ESTIMATE)
call fftw_execute_dft(plan, in, out)
call fftw_destroy_plan(plan)
```

Similarly, we can perform a inverse DFT by the following codes:

```
plan = fftw_plan_dft_1d(ngrids, in, out, FFTW_BACKWARD, FFTW_ESTIMATE)
call fftw_execute_dft(plan, in, out)
call fftw_destroy_plan(plan)
```

Note that the forward DFT in FFTW is defined by

$$H_n \equiv \sum_{j=0}^{N-1} h_j \exp\left(-\frac{2\pi i}{N} n j\right), \quad (64)$$

and the inverse DFT is defined by

$$h_j = \sum_{n=0}^{N-1} H_n \exp\left(\frac{2\pi i}{N} n j\right), \quad (65)$$

where there is no  $1/N$  factor in the inverse DFT, and thus this factor should be included by hand if we want to recover the original data from the inverse DFT.

## 4.10 Proof of the inverse DFT

In order to solve the linear algebraic equations (48) for  $h_j$ , multiply both sides of each equation by  $\exp\left(-\frac{2\pi i}{N} n J\right)$  and then add all the equations together, which yields

$$\sum_{n=0}^{N-1} \exp\left(-\frac{2\pi i}{N} n J\right) H_n = \sum_{n=0}^{N-1} \sum_{j=0}^{N-1} h_j \exp\left(\frac{2\pi i}{N} n(j-J)\right). \quad (66)$$

Interchanging the sequence of the two summation on the right-hand side, equation (66) is written

$$\sum_{n=0}^{N-1} \exp\left(-\frac{2\pi i}{N} n J\right) H_n = \sum_{j=0}^{N-1} h_j \sum_{n=0}^{N-1} \exp\left(\frac{2\pi i}{N} n(j-J)\right). \quad (67)$$

Using the fact that (verified by Wolfram Mathematica)

$$\sum_{n=0}^{N-1} \exp\left[\frac{i2\pi}{N} n(j-J)\right] = N\delta_{jJ}, \quad (68)$$

where  $\delta_{ij}$  is the Kroneker Delta, equation (67) is written

$$\sum_{n=0}^{N-1} \exp\left(-\frac{2\pi i}{N} nJ\right) H_n = \sum_{j=0}^{N-1} h_j N \delta_{jJ}, \quad (69)$$

i.e.,

$$\sum_{n=0}^{N-1} \exp\left(-\frac{2\pi i}{N} nJ\right) H_n = N h_J, \quad (70)$$

which can be solved to give

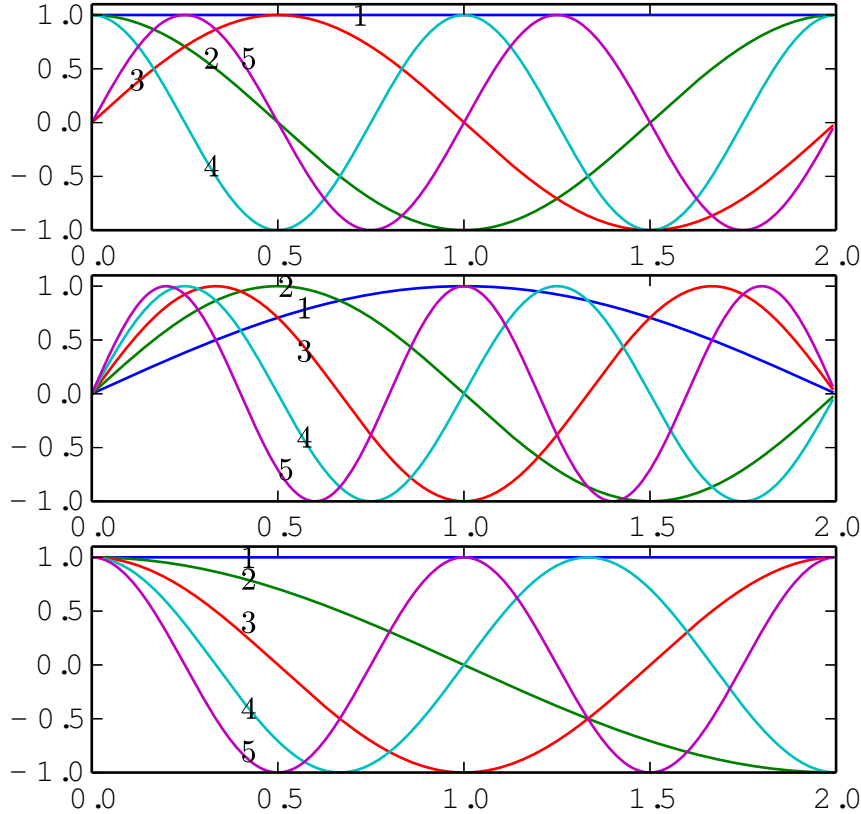
$$h_J = \frac{1}{N} \sum_{n=0}^{N-1} \exp\left(-\frac{2\pi i}{N} nJ\right) H_n. \quad (71)$$

Equation (71) is the inverse DFT.

## 5 Sine transform and Cosine transform

We mentioned (without giving proof) that the set of functions  $\cos(k\pi x/L)$  and  $\sin(k\pi x/L)$  with  $k=0, 1, \dots, \infty$  is a “complete set” in expanding any function in the interval  $(x_0, x_0 + 2L)$ , where  $x_0$  is an arbitrary point. Therefore Fourier series use both cosine and sine as basis functions to expand a function. Let us introduce another conclusion (again without giving proof) that the set of sine functions  $\sin(k\pi x/(2L))$  with  $k=1, 2, \dots, \infty$  is a “complete set” in expanding any function  $h$  in the interval  $(x_0, x_0 + 2L)$ . A similar conclusion is that the set of cosine functions  $\cos(k\pi x/(2L))$  with  $k=0, 1, 2, \dots, \infty$  is a “complete set” in expanding any function  $h$  in the interval  $(x_0, x_0 + 2L)$ . Note that the argument of the basis functions used in the Fourier expansion and the sine (or cosine) expansion differs by a factor of two, namely  $k\pi x/L$  and  $k\pi x/(2L)$ .

The first five basis functions used in Fourier expansion, sine expansion, and cosine expansion are plotted in Fig. 3.

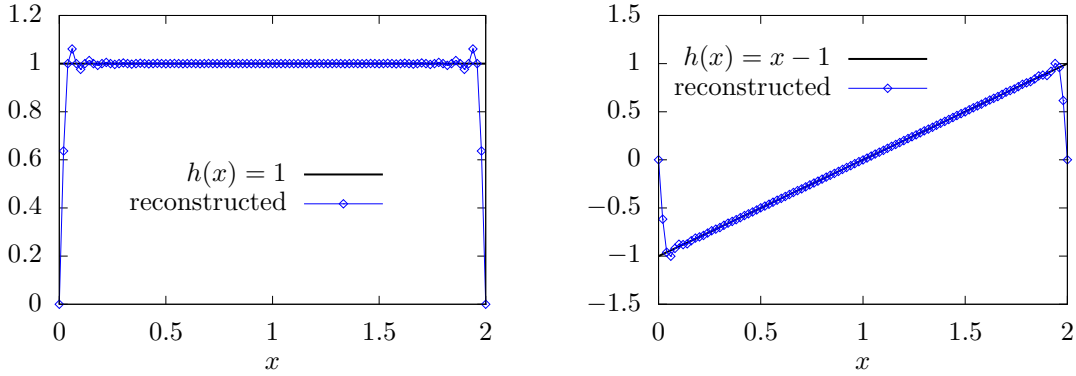


**Figure 3.** The first five basis functions used in Fourier expansion (upper), sine expansion (middle), and cosine expansion (lower) in the interval  $[x_0, x_0 + 2L]$  with  $x_0 = 0$  and  $L = 1$ .

The basis function  $b_k(x)$  used in the Fourier expansion have the properties  $b_k(x_0) = b_k(x_0 + 2L)$ . Therefore Fourier expansion works best for function that satisfy  $h(x_0) = h(x_0 + 2L)$ . For functions that do not satisfies this condition, there will be Gibbs oscillations near the interval boundary when approximated by using the Fourier expansion. A function with  $h(x_0) \neq h(x_0 + 2L)$  can be considered as a periodic function with period  $2L$  but having discontinuity points at the interval boundary. Gibbs oscillation appear near discontinuity points, which can be inner points in the interval or at the interval boundaries.

The basis functions  $b_k(x)$  used in sine expansion have the properties  $b_k(x_0) = b_k(x_0 + 2L) = 0$ . Therefore since expansion works best for functions that satisfy  $h(x_0) = h(x_0 + 2L) = 0$ . For functions that do not satisfies this condition, there will be Gibbs oscillations near the interval boundary when approximated by using the sine expansion. Examples are shown in Fig. 4.

The basis functions  $b_k(x)$  used in cosine expansion have the properties  $b'_k(x_0) = b'_k(x_0 + 2L) = 0$ . Therefore cosine expansion works best for functions that satisfy  $h'(x_0) = h'(x_0 + 2L) = 0$ . For functions that do not satisfies this condition, there will be Gibbs oscillations near the interval boundary when approximated by using the cosine expansion (to be verified numerically by me).



**Figure 4.** Left: constant function  $h(x) = 1$  approximated by using the sine expansion. Right: linear function  $h(x) = x - 1$  approximated by using the sine expansion. Gibbs oscillation appears near the boundaries, where  $h(x)$  does not satisfy the condition  $h(x_0) = h(x_0 + 2L) = 0$  ( $x_0 = 0$  and  $L = 1$  for this case). The expansion coefficients  $H_k$  are obtained via the discrete sine transform (72) with number of sampling point  $N = 50$ . The reconstruction formula is given by  $h(x) = \frac{2}{N} \sum_{k=1}^{N-1} H_k \sin\left(\frac{k\pi x}{2L}\right)$ .

Next, let us discuss the sine and cosine transformation.

### 5.1 Definition of the Discrete Sine Transform (DST)

There are many slightly different types of Discrete Sine Transforms (DST). One form I saw in W. Press's numerical recipe book is given by

$$H_k = \sum_{j=1}^{N-1} h_j \sin\left(\frac{k\pi j}{N}\right), \quad (72)$$

(which can be obtained formally by replacing DFT's exponential function by sine and the  $2\pi$  by  $\pi$ .) The inverse sine transformation is given by (I did not derive this, but has numerically verified that this transform recover the original data if applied after the sine transform (72))

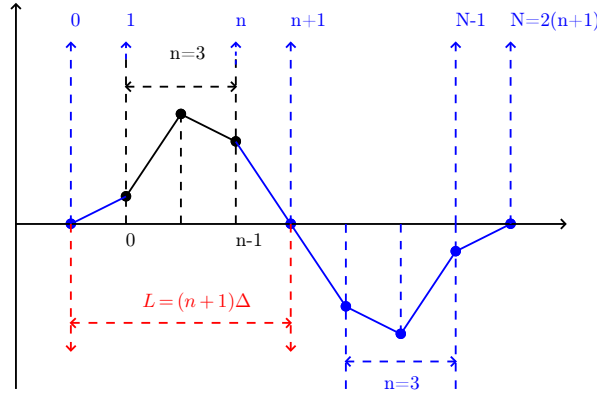
$$h_j = \frac{2}{N} \sum_{k=1}^{N-1} H_k \sin\left(\frac{k\pi j}{N}\right), \quad (73)$$

which is identical with the original transformation except for the normalization factor  $2/N$ .

Of course we need a fast method of computing the above DST. All fast methods for this finally need to make use of the fast method used in the computation of DFT. To conveniently use the fast method of DFT, we need carefully define the DST so that the DST can make easy connection to the DFT so that the DFT fast method can be easily applied to compute the DST. A standard way of making this easy is to define the DST via the DFT of a odd extension of the original data. Next, let us discuss this.

## 5.2 Define DST via DFT

Let us introduce the Discrete Sine Transform (DST) by odd extending a given real number sequence and then using the DFT of the extended data to define the DST. There are several slightly different way of odd extending a given sequence and thus different types of DST. Given a  $n = 3$  real number sequence  $(a, b, c)$ , one frequently adopted odd extension is  $(0, a, b, c, 0, -a, -b, -c, 0)$ . This odd extension is illustrated in Fig. 5.



**Figure 5.** Frequently used odd extension of real number sequence. The black points are original data (with index  $0, 1, \dots, n-1$ ). The blue points are introduced to generate an odd periodic sequence of numbers with index  $0, 1, \dots, N$ , where  $N = 2(n+1)$ . The point used in the DFT is  $0, 1, 2, \dots, N-1$ .

After the extension, the total number of points is  $N+1$  with  $N = 2(n+1)$ . Then DFT use the  $N$  points with index  $j = 0, 1, \dots, N-1$  as input. The output of this DFT is an odd symmetric sequence of purely imaginary numbers. Next, let us examine the output and try to simplify it. The DFT in this case is given by

$$H_k = \sum_{j=0}^{N-1} h'_j \exp\left(-\frac{2\pi i}{N} k j\right), \quad (74)$$

where  $h'_j$  is the odd extension of the original data  $h_j$ . For  $j = 1, 2, \dots, n$ , the relation between  $h'_j$  and  $h_j$  is given by

$$h'_j = h_{j-1}, \quad (75)$$

For  $j = n+2, \dots, N-1$ , the relation between  $h'_j$  and  $h_j$  is given by

$$h'_j = -h_{2n+1-j}. \quad (76)$$

Note that  $h'_0 = 0$  and  $h'_{n+1} = 0$ , then expression (74) is written as

$$H_k = 0 + \sum_{j=1}^n h'_j \exp\left(-\frac{2\pi i}{N} k j\right) + 0 + \sum_{j=n+2}^{N-1} h'_j \exp\left(-\frac{2\pi i}{N} k j\right). \quad (77)$$

Using  $N = 2(n+1)$ , the above expression is written as

$$H_k = \sum_{j=1}^n h'_j \exp\left(-\frac{\pi i}{(n+1)} k j\right) + \sum_{j=n+2}^{2n+1} h'_j \exp\left(-\frac{\pi i}{(n+1)} k j\right) \quad (78)$$

Using the relations (75) and (76) to replace  $h'_j$  by  $h_j$ , the above expression is written

$$H_k = \sum_{j=1}^n h_{j-1} \exp\left(-\frac{\pi i}{(n+1)} k j\right) - \sum_{j=n+2}^{2n+1} h_{2n+1-j} \exp\left(-\frac{\pi i}{(n+1)} k j\right). \quad (79)$$

Change the definition of the dump index  $j$  in the above summation to make it in the conventional range  $[0: n-1]$ , the above expression is written as

$$H_k = \sum_{j=0}^{n-1} h_j \exp\left(-\frac{\pi i}{(n+1)} k(j+1)\right) - \sum_{j=0}^{n-1} h_{n-1-j} \exp\left(-\frac{\pi i}{(n+1)} k(j+n+2)\right).$$

Defining  $j' = n-1-j$  to replace the dump index in the second summation, the above expression is written as

$$\begin{aligned} H_k &= \sum_{j=0}^{n-1} h_j \exp\left(-\frac{\pi i}{(n+1)} k(j+1)\right) - \sum_{j'=n-1}^0 h_{j'} \exp\left(-\frac{\pi i}{(n+1)} k(2n+1-j')\right) \\ &= \sum_{j=0}^{n-1} h_j \exp\left(-\frac{\pi i}{(n+1)} k(j+1)\right) - \sum_{j=0}^{n-1} h_j \exp\left(-\frac{\pi i}{(n+1)} k(2n+1-j)\right) \\ &= \sum_{j=0}^{n-1} h_j \exp\left(-\frac{\pi i}{(n+1)} k(j+1)\right) - \sum_{j=0}^{n-1} h_j \exp\left(-\frac{\pi i}{(n+1)} k(-j-1)\right) \\ &= -2i \sum_{j=0}^{n-1} h_j \sin\left(\frac{\pi}{(n+1)} k(j+1)\right), \end{aligned} \quad (80)$$

which is a purely imaginary number. Expression (80) has the symmetry

$$H_{N-k} = -H_k, \quad (81)$$

which is called odd symmetry. Therefore only half of the data for  $H_k$  with  $k = 0, 1, \dots, N-1$  need to be stored, namely  $H_k$  with  $k = 0, 1, \dots, N/2$ . Equations (81) indicates that  $H_0$  and  $H_{N/2}$  are definitely zero and thus do not need to be stored. Then the remaining data to be stored are  $H_k$  with  $k = 1, 2, \dots, N/2-1$ , i.e.,  $H_k$  with  $k = 1, 2, \dots, n$ . Following the convention of making the index of  $H_k$  in the range  $[0: n-1]$ , we define  $H'_k = H_{k+1}$ . Then

$$H'_k = -2i \sum_{j=0}^{n-1} h_j \sin\left(\frac{\pi}{(n+1)} (k+1)(j+1)\right) \quad (82)$$

with  $k = 0, 1, 2, \dots, n-1$ , which is the index that we prefer. Finally, the so-called type-I Discrete Sine Transform (DST-I) is defined based on Eq. (82) via

$$Y_k = \frac{H_{k+1}}{-i} = \frac{H'_k}{-i} = 2 \sum_{j=0}^{n-1} h_j \sin\left(\frac{\pi}{(n+1)} (k+1)(j+1)\right), \quad (83)$$

with  $k = 0, 1, 2, \dots, n-1$ .

### 5.3 The meaning of DST

From the above derivation, we know that the DST,  $Y_k$ , is related to the DFT,  $H_k$ , by  $Y_k = H_{k+1}/(-i)$ , and thus the meaning of  $Y_k$  is in principle clear.

Next, let us examine the meaning of the DST in more details so that we can easily use it in practice. Let us try to use the DST to reconstruct a function that approximates the original data. Since DST is only a special case of DFT, reconstruct the function using DST follows the same procedure used in DFT. In DFT, the function that approximates the original data is reconstructed via Eq. (61) (changing to the positive exponent convention), i.e.,

$$h(x) = \frac{1}{N} \left[ \sum_{k=0}^{N/2} H_k e^{ik2\pi x/(2L)} + \sum_{k=N/2}^{N-1} H_k e^{i(k-N)2\pi x/(2L)} \right]. \quad (84)$$

where  $2L$  is the length of the interval in which the samplings  $h_j$  with  $j = 0, 1, \dots, N - 1$  are made. For our present case, i.e., an odd extension of the original  $n$  data, we have  $N = 2(n + 1)$  and  $H_0 = 0$  and  $H_{N/2} = 0$ . Then Eq. (84) is written as

$$h(x) = \frac{1}{N} \left[ 0 + \sum_{k=1}^n H_k e^{ik2\pi x/(2L)} + 0 + \sum_{k=n+2}^{2n+1} H_k e^{i(k-N)2\pi x/(2L)} \right]. \quad (85)$$

Using the odd symmetry of  $H_k$ , i.e.,  $H_k = -H_{N-k}$ , the above expansion is written as

$$h(x) = \frac{1}{N} \left[ \sum_{k=1}^n H_k e^{ik2\pi x/(2L)} - \sum_{k=n+2}^{2n+1} H_{N-k} e^{i(k-N)2\pi x/(2L)} \right]. \quad (86)$$

Define  $k' = 2n + 2 - k$ , and note that  $N = 2(n + 1)$ , then the above expression is written as

$$h(x) = \frac{1}{2(n+1)} \left[ \sum_{k=1}^n H_k e^{ik2\pi x/(2L)} - \sum_{k'=n}^1 H_{k'} e^{i(-k')2\pi x/(2L)} \right]. \quad (87)$$

i.e.,

$$h(x) = \frac{1}{2(n+1)} \sum_{k=1}^n H_k (e^{ik2\pi x/(2L)} - e^{-ik2\pi x/(2L)}), \quad (88)$$

which is simplified as

$$h(x) = \frac{1}{2(n+1)} \sum_{k=1}^n 2i H_k \sin\left(\frac{k2\pi x}{2L}\right). \quad (89)$$

As a convention, we prefer that the summation index begins from 0 and ends at  $n - 1$ . Then expression (89) is re-written as

$$h(x) = \frac{1}{2(n+1)} \sum_{k=0}^{n-1} 2i H_{k+1} \sin\left(\frac{(k+1)2\pi x}{2L}\right)$$

Using the relation between DST and DFT, i.e.,  $H_{k+1} = -iY_k$ , the above equation is written as

$$h(x) = \frac{1}{n+1} \sum_{k=0}^{n-1} Y_k \sin\left(\frac{(k+1)2\pi x}{2L}\right). \quad (90)$$

This is the formula for constructing a function approximating the original function using the DST data. This formula is a expansion over the basis functions  $\sin[(k+1)\pi x/L]$  with the DST  $Y_k$  acting as the expansion coefficients. Therefore the direct meaning of the DST,  $Y_k$ , is that they are the expansion coefficients when using the sine functions  $\sin[(k+1)\pi x/L]$  as the basis functions to approximate a function in the interval of length  $L$ . From Fig. 5, we know that the interval length  $L$  is given by  $L = (n - 1)\Delta + 2\Delta = (n + 1)\Delta$ , where  $\Delta$  is the uniform interval of the original  $n$  sampling points.

## 5.4 Discrete Cosine transform

to be written

# 6 Misc content

## 6.1 Multi-dimensional Fourier series

Compared with Eq. (1) that uses the trigonometric functions, Fourier series (11) and (12), which is expressed in terms of the complex exponential function  $e^{in\pi x/L}$ , is more compact. The convenience introduced by the complex exponential function can be more easily appreciated when we deal with multiple-dimensional Fourier series. For example, a two-dimensional function  $G(x, y)$  can be expanded as Fourier series about  $x$ ,

$$G(x, y) = \sum_{m=-\infty}^{\infty} c_m(y) e^{im\pi x/L_x}, \quad (91)$$

where  $2L_x$  is the period of  $G$  in  $x$  direction. The expansion coefficients  $c_m(y)$  can be further expanded as Fourier series about  $y$ ,

$$c_m(y) = \sum_{n=-\infty}^{\infty} (c_{mn} e^{in\pi y/L_y}), \quad (92)$$

where  $2L_y$  is the period of  $G$  in  $y$  direction. Using Eq. (92) in Eq. (91), we obtain

$$G(x, y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} c_{mn} e^{in\pi y/L_y + im\pi x/L_x}, \quad (93)$$

where the coefficients  $c_{mn}$  can be written

$$\begin{aligned} c_{mn} &= \frac{1}{2L_y} \int_{-L_y}^{L_y} \left[ \frac{1}{2L_x} \int_{-L_x}^{L_x} G(x, y) e^{-im\pi x/L_x} dx \right] e^{-in\pi y/L_y} dy. \\ &= \frac{1}{4L_x L_y} \int_{-L_y}^{L_y} \int_{-L_x}^{L_x} G(x, y) e^{-im\pi x/L_x - in\pi y/L_y} dx dy. \end{aligned} \quad (94)$$

Equations (93) and (94) give the two-dimensional Fourier series of  $G(x, y)$ . We see that the extension of Fourier series from one-dimension case to two-dimension case is straightforward when expressed in terms of the complex exponential function  $e^{in\pi x/L}$ . However, if we use  $\sin(m\pi x/L_x)$ ,  $\cos(m\pi x/L_x)$ ,  $\sin(n\pi y/L_y)$ , and  $\cos(n\pi y/L_y)$  as basis functions, the two-dimensional Fourier series of  $G(x, y)$  is a little complicated (refer to Sec. 6.2). The final result is given by

$$G(x, y) = \sum_{n=-\infty}^{\infty} \sum_{m=0}^{\infty} \left[ G_{nm}^c \cos\left(\frac{m\pi x}{L_x} + \frac{n\pi y}{L_y}\right) + G_{nm}^s \sin\left(\frac{m\pi x}{L_x} + \frac{n\pi y}{L_y}\right) \right], \quad (95)$$

where the coefficient  $G_{00}^c$  is given by

$$G_{00}^c = \frac{1}{4L_x L_y} \int_{-L_y}^{L_y} \int_{-L_x}^{L_x} G(x, y) dx dy. \quad (96)$$

and other coefficients are given by

$$G_{nm}^c = \frac{1}{2L_x L_y} \int_{-L_y}^{L_y} \int_{-L_x}^{L_x} G(x, y) \cos\left(\frac{m\pi x}{L_x} + \frac{n\pi y}{L_y}\right) dx dy. \quad (97)$$

$$G_{nm}^s = \frac{1}{2L_x L_y} \int_{-L_y}^{L_y} \int_{-L_x}^{L_x} G(x, y) \sin\left(\frac{m\pi x}{L_x} + \frac{n\pi y}{L_y}\right) dx dy. \quad (98)$$

## 6.2 Multidimensional Fourier series using trigonometric functions cosine and sine

This section is to demonstrate that multiple-dimensional Fourier series will become complicated if we use the cosine and sine as basis functions. A two-dimensional function  $G(x, y)$  can be first expanded as Fourier series about  $x$ ,

$$G(x, y) = \sum_{m=0}^{\infty} a_m(y) \cos\left(\frac{m\pi}{L_x} x\right) + \sum_{m=0}^{\infty} b_m(y) \sin\left(\frac{m\pi}{L_x} x\right), \quad (99)$$

and then the two coefficients  $a_m(y)$  and  $b_m(y)$  can be further expanded as Fourier series about  $y$ ,

$$a_m(y) = \sum_{n=0}^{\infty} a_{mn}^{(a)} \cos\left(\frac{n\pi}{L_y} y\right) + \sum_{n=0}^{\infty} b_{mn}^{(a)} \sin\left(\frac{n\pi}{L_y} y\right), \quad (100)$$

$$b_m(y) = \sum_{n=0}^{\infty} a_{mn}^{(b)} \cos\left(\frac{n\pi}{L_y} y\right) + \sum_{n=0}^{\infty} b_{mn}^{(b)} \sin\left(\frac{n\pi}{L_y} y\right), \quad (101)$$



Substituting Eq. (100) and (101) into Eq. (99), we obtain

$$\begin{aligned} G(x, y) = & \sum_{m=0}^{\infty} \left[ \sum_{n=0}^{\infty} a_{mn}^{(a)} \cos\left(\frac{n\pi}{L_y} y\right) + \sum_{n=0}^{\infty} b_{mn}^{(a)} \sin\left(\frac{n\pi}{L_y} y\right) \right] \cos\left(\frac{m\pi}{L_x} x\right) \\ & + \sum_{m=0}^{\infty} \left[ \sum_{n=0}^{\infty} a_{mn}^{(b)} \cos\left(\frac{n\pi}{L_y} y\right) + \sum_{n=0}^{\infty} b_{mn}^{(b)} \sin\left(\frac{n\pi}{L_y} y\right) \right] \sin\left(\frac{m\pi}{L_x} x\right). \end{aligned} \quad (102)$$

Next, we consider the special case that  $2L_x = 2L_y = 2\pi$  and use  $\theta$  and  $\phi$  to denote  $x$  and  $y$ , respectively. Then Eq. (102) is written

$$\begin{aligned} G(\theta, \phi) = & \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} a_{mn}^{(a)} \cos(n\phi) \cos(m\theta) + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} b_{mn}^{(a)} \sin(n\phi) \cos(m\theta) \\ & + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} a_{mn}^{(b)} \cos(n\phi) \sin(m\theta) + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} b_{mn}^{(b)} \sin(n\phi) \sin(m\theta), \end{aligned} \quad (103)$$

Using the product-to-sum trigonometric identities, equation (103) is written

$$\begin{aligned} G(\theta, \phi) = & \frac{1}{2} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} a_{mn}^{(a)} [\cos(m\theta + n\phi) + \cos(m\theta - n\phi)] + \frac{1}{2} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} b_{mn}^{(a)} [\sin(m\theta + n\phi) - \sin(m\theta - n\phi)] \\ & + \frac{1}{2} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} a_{mn}^{(b)} [\sin(m\theta + n\phi) + \sin(m\theta - n\phi)] + \frac{1}{2} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} b_{mn}^{(b)} [\cos(m\theta - n\phi) - \cos(m\theta + n\phi)] \\ = & \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{1}{2} [a_{mn}^{(a)} - b_{mn}^{(b)}] \cos(m\theta + n\phi) + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{1}{2} [b_{mn}^{(a)} + a_{mn}^{(b)}] \sin(m\theta + n\phi) \\ & + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{1}{2} [a_{mn}^{(a)} + b_{mn}^{(b)}] \cos(m\theta - n\phi) + \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{1}{2} [-b_{mn}^{(a)} + a_{mn}^{(b)}] \sin(m\theta - n\phi) \end{aligned} \quad (104)$$

Equation (104) is obviously more complicated than Eq. (93) that uses complex exponential functions. (It is ready to realize that the Fourier series will become even complicated for the three-dimensional case.) The coefficients appearing in Eq. ( ) are written

$$a_m(y) = \frac{1}{L_x} \int_{-L_x}^{-L_x} G(x, y) \cos\left(\frac{m\pi}{L_x} x\right) dx \quad (105)$$

$$b_m(y) = \frac{1}{L_x} \int_{-L_x}^{-L_x} G(x, y) \sin\left(\frac{m\pi}{L_x} x\right) dx \quad (106)$$

$$a_{mn}^{(a)} = \frac{1}{L_x} \frac{1}{L_y} \int_{-L_y}^{-L_y} \int_{-L_x}^{-L_x} G(x, y) \cos\left(\frac{m\pi}{L_x} x\right) \cos\left(\frac{n\pi}{L_y} y\right) dx dy \quad (107)$$

$$a_{mn}^{(b)} = \frac{1}{L_x} \frac{1}{L_y} \int_{-L_y}^{-L_y} \int_{-L_x}^{-L_x} G(x, y) \cos\left(\frac{m\pi}{L_x} x\right) \sin\left(\frac{n\pi}{L_y} y\right) dx dy \quad (108)$$

$$b_{mn}^{(a)} = \frac{1}{L_x} \frac{1}{L_y} \int_{-L_y}^{-L_y} \int_{-L_x}^{-L_x} G(x, y) \sin\left(\frac{m\pi}{L_x} x\right) \cos\left(\frac{n\pi}{L_y} y\right) dx dy \quad (109)$$

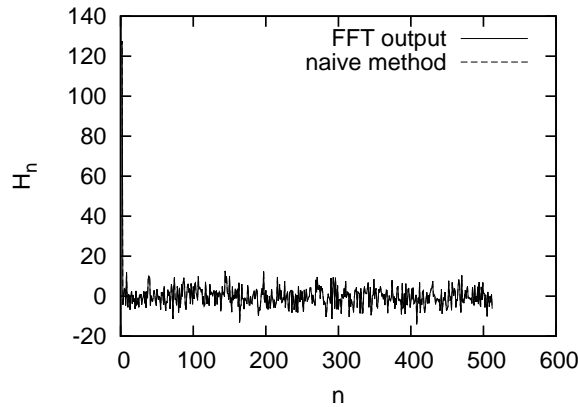
$$b_{mn}^{(b)} = \frac{1}{L_x} \frac{1}{L_y} \int_{-L_y}^{-L_y} \int_{-L_x}^{-L_x} G(x, y) \sin\left(\frac{m\pi}{L_x} x\right) \sin\left(\frac{n\pi}{L_y} y\right) dx dy \quad (110)$$

### 6.3 Details on FFT codes provided by the Numerical recipes book[2]

The following is about a specific FFT subroutine provided by the Numerical recipes book[2]. This is not a general case.

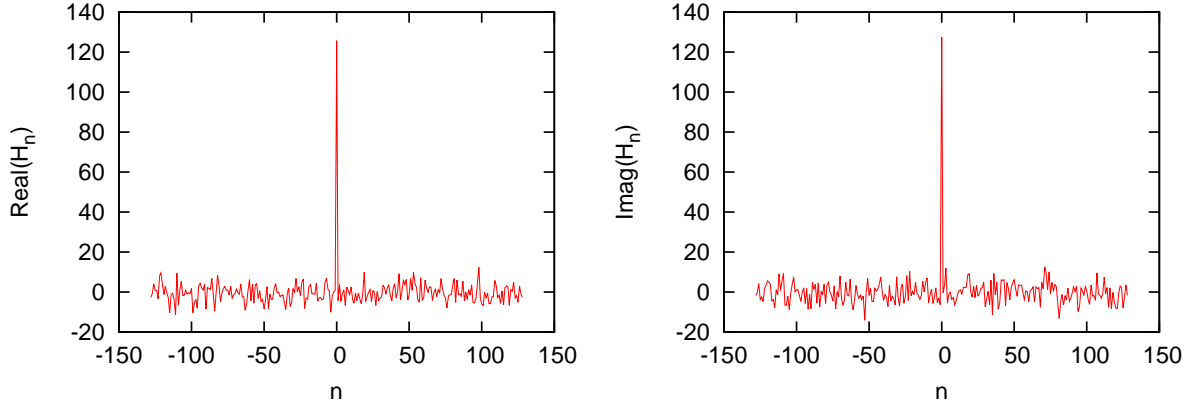
The input and output of the DFT are usually complex numbers. In the implementation of FFT algorithm provided by Numerical recipes book[2], to avoid using complex numbers, the algorithm adopts the real number representation of the complex numbers. In this scheme, two elements of a real number array are used to store one complex number. To store a complex array “cdata” of length  $N$ , we will need a real number array “rdata” of length  $2N$ . The first elements of array “rdata” will contain the real part of “cdata(1)”, the second elements of “rdata” will contain the imaginary part of “cdata(1)”, and so on.

To test the correctness of the above statement, I generated a real number array with length  $N = 2 \times 2^8$  by using a random generating routine and calculate the DFT of the array with two methods. The real array generated by the random generator are considered to be a real number representation of a complex array with length  $N/2$ . Using the real array as the input of the FFT routine (the code in `~/project_new/fft`). To check the correctness of my understanding of the input and output of the FFT, I manually convert the real number of length  $N$  to a complex array with length  $N/2$ , and use directly the summation in Eq. (50) to calculate the DFT. The output I got is obviously a complex array with length  $N/2$ . Then I manually convert the complex array to a real number array of length  $N$  and plot the output in Fig. 6 with dashed line. The results in Fig. 6 indicates the results given by the FFT and the naive method used by me agree with each other well. This proves that my understanding of the input and output of FFT (especially the storage arrangement) is correct.



**Figure 6.** The output of a FFT routine (solid line) agrees well with those (dashed line) calculated by directly evaluate the summation in Eq. (50) (the latter is coded by me). The agreement indicates my understanding of the output of FFT (especially the storage arrangement) is correct. Here the time domain data is generated by a random generating routine.

To clearly show the output of FFT, we recover the real and imaginary part of DFT from the output of FFT and plots the data as a function of their corresponding frequency. The results are given in Fig. 7.



**Figure 7.** The real (left) and imaginary (right) part of the discrete Fourier transformation as a function of the frequency. The point  $n = -128$  corresponds to frequency  $-f_s/2$  while the point  $n = 128$  corresponds to frequency  $+f_s/2$ , where  $f_s = 1/\Delta$  with  $\Delta$  is the sample interval in time domain. The time domain data is the same as used in Fig. 6. Why is there a spike at zero frequency?

## 6.4 Computing Fourier integrals using FFT (not finished, to be deleted)

Consider the calculation of the following integral:

$$I(\omega) = \int_a^b e^{i\omega t} h(t) dt. \quad (111)$$

Divide the interval  $[a, b]$  into  $M$  uniform sub-intervals and define

$$\Delta = \frac{b-a}{M}, t_j = a + \Delta j, h_j = h(t_j), j = 0, 1, 2, \dots, M \quad (112)$$

Then the integration in Eq. (111) can be approximated as

$$I(\omega) \approx \Delta \sum_{j=0}^{M-1} h_j \exp(i\omega t_j). \quad (113)$$

Define  $\omega_m = 2\pi m / (M\Delta)$  with integer  $m$  and  $-M/2 < m < M/2$ . Consider the calculation of  $I(\omega_m)$ . Using Eq. (113), we obtain

$$\begin{aligned} I(\omega_m) &= \Delta \sum_{j=0}^{M-1} h_j \exp[i\omega_m(a + \Delta j)] \\ &= \Delta e^{i\omega_m a} \sum_{j=0}^{M-1} h_j \exp(i\omega_m \Delta j) \\ &= \Delta e^{i\omega_m a} \sum_{j=0}^{M-1} h_j \exp\left(i \frac{2\pi m}{M} j\right) \\ &= \Delta e^{i\omega_m a} H_m \end{aligned} \quad (114)$$

$$= \Delta e^{i\omega_m a} [\text{DFT}(h_0, h_1, h_2, \dots, h_{M-1})]_m. \quad (115)$$

Equation (115) indicates the value of the integration  $I(\omega_m)$  can be obtained by calculating the discrete Fourier transformation of  $h_j$ . However, as discussed in Ref. [2], equation (115) is not recommended for practical use because the oscillatory nature of the integral will make Eq. (115) become systematically inaccurate as  $\omega$  increases. Next, consider a new method, in which  $h(t)$  is expanded as

$$h(t) \approx \sum_{j=0}^M h_j \psi\left(\frac{t-t_j}{\Delta}\right) + \sum_{j=\text{endpoints}} h_j \varphi_j\left(\frac{t-t_j}{\Delta}\right) \quad (116)$$

Apply the integral operator  $\int_a^b dt \exp(i\omega t)$  to both sides of Eq. (116), we obtain

$$\int_a^b h(t) e^{i\omega t} dt \approx \sum_{j=0}^M h_j \int_a^b \psi\left(\frac{t-t_j}{\Delta}\right) e^{i\omega t} dt + \sum_{j=\text{endpoints}} h_j \int_a^b \varphi_j\left(\frac{t-t_j}{\Delta}\right) e^{i\omega t} dt. \quad (117)$$

Make the change of variables  $s = (t - t_j) / \Delta$  in the first integral and  $s = (t - a) / \Delta$  in the second integral, the above equation is written as

$$\int_a^b h(t) e^{i\omega t} dt \approx \Delta \sum_{j=0}^M h_j \int_a^b \psi(s) e^{i\omega(\Delta s + t_j)} ds + \Delta \sum_{j=\text{endpoints}} h_j \int_a^b \varphi_j(s - j) e^{i\omega(\Delta s + a)} ds \quad (118)$$

Define  $\theta = \omega \Delta$  and make use of  $t_j = a + j\Delta$ , the above equation is written as

$$\int_a^b h(t) e^{i\omega t} dt \approx \Delta e^{i\omega a} \sum_{j=0}^M h_j e^{i\theta j} \int_a^b \psi(s) e^{i\theta s} ds + \Delta e^{i\omega a} \sum_{j=\text{endpoints}} h_j \int_a^b \varphi_j(s - j) e^{i\theta s} ds \quad (119)$$

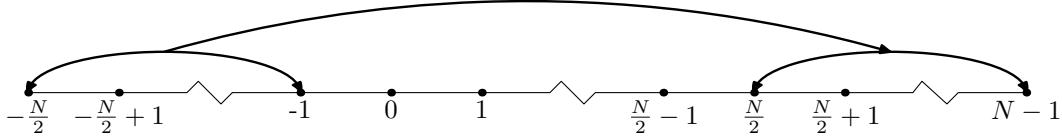
Define

$$W(\theta) = \int_a^b \psi(s) e^{i\theta s} ds \quad (120)$$

$$\alpha_j(\theta) = \int_a^b \varphi_j(s - j) e^{i\theta s} ds \quad (121)$$

Then Eq. (119) is written as

$$\int_a^b h(t) e^{i\omega t} dt \approx \Delta e^{i\omega a} \left[ W(\theta) \sum_{j=0}^M h_j e^{i\theta j} + \sum_{j=\text{endpoints}} h_j \alpha_j(\theta) \right]. \quad (122)$$



**Figure 8.** Older version of Fig. 2, created by Metapost, the new version is created by the vector graphic editor in TeXmacs.

## Bibliography

- [1] *A Guided Tour of Mathematical Physics*. Samizdat Press, 1994.
- [2] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery. *Numerical Recipes in Fortran 77*. Cambridge University Press, Cambridge, UK, 1992.