Submitted to JVSTA

A Tutorial on the Fourier Transform and Discrete Fourier Transform in the Context of Denoising Spectra

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I. ABSTRACT

In another article in this special collection (*J. Vac. Sci.Technol. A,* **2025**, *43*, 033401), we made the case for the Fourier denoising of X-ray photoelectron spectroscopy (XPS) data. We believe that this capability will be useful when it is not possible to collect the best possible data and when the data are to be used for artificial intelligence (AI) applications, as noise tends to confuse AI algorithms. Nevertheless, while Fourier analysis appears to be the most powerful way for removing noise from data, some who might like to use it are not experts in it. This document describes the Fourier transform (FT) and discrete Fourier transform (DFT) in both general and specific ways in the context of denoising spectra. That is, after some introductory words, which motivate the topic, it first provides enough information to the future user to be able to denoise many spectra in a reasonable fashion. Thereafter, it covers some of the mathematical theory of the Fourier transform and discrete Fourier transform. Even a partial understanding of this material will help those who wish to use Fourier theory to use it more successfully. The Fourier transform and discrete Fourier transform are powerful tools for data analysis.

II. MOTIVATION

X-ray photoelectron spectrometer (XPS) manufacturers are making high-quality instruments that can collect enormous amounts of data. This data is useful for many purposes. It informs research and provides quality control for industrial processes. However, given the finite time, money, and human effort available for projects, it is often not possible to collect the best possible XPS data from specimens. Furthermore, the samples themselves can limit the quality of the data that can be obtained from them if they have analytes in very low concentrations or are damaged by an analysis. Of course, imperfect data is not always an issue. A trained analyst can often successfully interpret spectra with modest amounts of noise on them. However, this is not necessarily the case for Artificial Intelligence (AI) algorithms, which are often confused by noise. It can take considerably more noisy data to train an AI algorithm than noise-free data, and there is increasing interest in using surface analysis data in AI algorithms to control and understand deposition processes.

Recently, Linford, Aspnes, and coworkers made the case for the Fourier denoising of XPS data.[1] First, they showed that the Fourier approach is superior to traditional Savitzky-Golay and boxcar smooths.[2] In addition, surprisingly, they showed that smoothed spectra are often closer to the true underlying spectra than the unsmoothed spectra.

So far, as gauged by responses to presentations at conferences and in personal conversations with other experts, the XPS community has been receptive to the idea of the Fourier denoising of its data. Nevertheless, these interactions have also revealed that not everyone in the community is an expert in Fourier analysis. This lack of knowledge can have consequences. The inappropriate application of Fourier analysis to data can significantly distort it.[1]

The purpose of this tutorial is to provide the XPS community, and also scientists from other disciplines who may wish to use Fourier analysis, the basics of Fourier theory. It is the authors' experience that a deeper foundation in Fourier theory is valuable in applying it more successfully. Furthermore, there is an inherent beauty and elegance to Fourier theory.

This article covers both the Fourier transform (FT), which is used for continuous functions, and the discrete Fourier transform (DFT), which is used for discrete data, e.g., spectra. It should lay a reasonable foundation for the application of Fourier analysis to data smoothing. Counterintuitively, for many, the integrals in the Fourier analysis of continuous functions are easier to understand than the sums in the discrete Fourier transform. The Fourier analysis of continuous functions is thus a good starting point for learning the key principles of Fourier analysis that apply directly to data smoothing with the discrete Fourier transform. Accordingly, this article begins with the Fourier transform and then discusses the discrete Fourier transform.

III. FIRST AUTHOR'S PERSONAL NOTE

The Mayflower set sail from Plymouth, England in 1620 for America. It was filled with passengers of a persecuted minority seeking religious freedom. It is estimated that the original passengers of the Mayflower who survived and had children now have tens of millions of living descendants. These enormous numbers, no doubt driven by near exponential growth initially, are like estimates that, for example, most, if not all, English people today are descendants of William the Conqueror who, with dubious claims, sacked England in 1066. Did you know, for example, that there were already great cathedrals in England before 1066, but that William, tragically, had them torn down and rebuilt in the Norman style? Apparently, at least according to William, the history of England needed to start, or restart, with his conquest. Similarly, the women accused of witchcraft in the Salem Witch Trials of 1692 – 1693, which were a sham – these women were never witches, are estimated now to have enormous posterities – perhaps 15 million people. Some years ago, Linford's mother-in-law, who has ancestors that go back to Colonial America, discovered that she is a descendent of two of the women who were convicted of witchcraft and executed in the Salem witch trials: Bridgit Bishop and Rebecca Nurse. Bishop, a midwife, was the first woman put to death in these trials. She was hanged. Perhaps her only real 'crime' was that she may have been a little eccentric and was therefore a target of suspicion. Humorously, at the time this discovery was made about his wife's genealogy, Linford mentioned to a friend that his mother-in-law had recently discovered that she is descended from two witches. The friend said to Linford: "I wouldn't even touch that one." Ah, yes, another mother-in-law joke…

The previous paragraph may seem like a non sequitur for an article on the Fourier transform, but it is not. In the Salem witch trials, and at other such trials of 'witches', 'spectral evidence' was presented. Obviously, this term would mean something quite different in a modern trial. 'Spectral evidence' previously referred to supernatural occurrences associated with the accused witch. The idea was that somehow a spectral image of a witch could act in nefarious ways separate from the witch herself. The etymology of the word 'spectrum' is largely forgotten in modern science. It has the same root as the word 'specter', i.e., ghost or apparition. Many of us are familiar with Daniel Craig's James Bond movie 'Spectre', which uses the British spelling for this word. As an aside, recognizing that false evidence had been brought against the women convicted in the Salem Witch Trials, the descendants of the accusers in these trials have apologized on multiple occasions over the years to the descendants of the 'witches'. These trials were a serious matter, although 'Monte Python and the Holy Grail' seemed to have fun mocking the ideas behind them. In any case, the point here is that a spectrum, as we think about it, is distantly connected to the idea that it is somehow a visual representation or ghost of an object we wish to study. There is the object under study and there is the 'ghost' of it, a spectrum, which somehow represents it in a way like, perhaps, Hamlet's father, as a ghost, represented the dead king.

Thus, in spectroscopy, there is a duality, or division into two parts, of an object and its spectral representation. We are surrounded by dualities, both in science and otherwise. Here are three in science. A molecule or molecular fragment is either charged, or it is not, where this duality matters a lot in mass spectrometry. The (perpetual motion?) machine you are trying to patent either violates a law of thermodynamics, or it doesn't, where in the former case your application should be rejected. Of course, there is the wave-particle duality of quantum mechanics that captures the idea that very small particles exhibit some of the properties of both macroscopic waves and macroscopic particles. Here are three dualities outside of science. The first two involve some humor. First, when you speak with another person in German, you either use the formal 'Sie' or the informal 'du' for 'you'. Years ago, one of Linford's German friends explained his use of these personal pronouns. As he put it: "I use 'Sie' with people I don't like." Second, while fewer people smoke worldwide than did in the past, many people now vape. Accordingly, there are places in this world where Linford has thought: "There are only two types of people in this city: Those that smoke, and those that vape." Third, many religions, including the ancient Greeks, believe/believed in a spirit-body duality. You're either dead and in a spirit realm or you're alive. Or, as the King James Bible puts it so poetically, there are the 'quick and the dead'.

In this tutorial we describe a powerful mathematical duality that is created by Fourier analysis. Fourier analysis, especially with the discrete Fourier transform, has rightfully become one of the most widely used and most powerful tools for spectral analysis. Fourier analysis creates another representation of a spectrum (a ghost of a ghost perhaps?) in a reciprocal domain. In other words, Fourier analysis creates a dichotomy of information, expanding a spectrum into a second, mathematically equivalent, representation of it, which naturally emphasizes and reveals aspects of the spectrum that are often not as apparent or accessible in its direct space representation. One can choose the most advantageous domain to work in for a given problem.

Fourier analysis has been important for some time. At the beginning of a book on the Fourier transform, which, parenthetically, is a special case of the more general Laplace transform and is related to other transforms like the Hartley transform,[3, 4] Bracewell quotes Lord Kelvin who wrote: "Fourier's theorem is not only one of the most beautiful results of modern analysis, but it may be said to furnish an indispensable instrument in the treatment of nearly every recondite question in modern physics."

The intertwined and highly beneficial connections between the direct and reciprocal space representations of spectra and data offered by Fourier analysis are reminiscent of words from the Doctrine and Covenants,[5] which read:

> 33. For man is spirit. The elements are eternal, and spirit and element, inseparably connected, receive a fulness of joy;
>
> 34. And when separated, man cannot receive a fulness of joy.

IV. INTRODUCTION

Together, the Fourier transform, Fourier series, and discrete Fourier transform, i.e., Fourier analysis, constitute one of the most important mathematical advances of all time. They are also one of the most powerful and practical mathematical tools used by engineers, physicists, and other scientists. In real-world applications, Fourier analysis shows up wherever there are waves, signals, or spectra. Ultimately, Fourier analysis reveals the frequency content of spectra and signals. Entire chemical and material characterization methods are based on Fourier analysis, including Fourier transform infrared spectroscopy (FTIR), nuclear magnetic resonance, and Fourier-transform ion cyclotron resonance (FT-ICR) mass spectrometry. Fourier analysis is also at the heart of modern digital signal processing.

Spectra and signals of a wide variety are collected in science and engineering, where these spectra usually consist of both an underlying signal, which is generally considered to be the information of interest, and noise, which is usually viewed as masking or distorting the true signal. Assuming reasonable assumptions hold, Fourier analysis produces a mathematically equivalent domain in which to view a signal and the noise associated with it. It is often difficult, or even impossible, to fully understand a spectrum or signal without considering it in both domains. We refer to the domain in which the spectrum is taken, i.e., the domain in which it is traditionally displayed, as real or direct space and the domain created by the Fourier transform as indirect or reciprocal space.

One of the powerful features of Fourier analysis is that, in reciprocal space, it often separates the information and noise in a spectrum from each other, where the information of interest is generally contained in the lower-frequency Fourier coefficients, while the noise appears in the higher-frequency Fourier coefficients. This separation of signal and noise suggests a strategy for removing noise from data, where this possibility is both aided and allowed by a powerful theorem known as the convolution theorem. The convolution theorem, which will be discussed in this tutorial, teaches that multiplication in one domain (either domain) is equivalent to convolution in the other. Thus, via the convolution theorem, one may multiply the Fourier coefficients of a spectrum in the reciprocal domain by a function known as a transfer or filter function. In general, this multiplication can effectively preserve the real information in the spectrum, while removing a significant fraction of the noise from it. After this multiplication, the resulting, modified Fourier coefficients are back transformed into direct space. This approach is equivalent to applying a smooth to the data as a convolution in direct space. If a reasonable transfer function is selected and appropriately placed on the Fourier coefficients in reciprocal space, and if, to begin with, the spectrum follows the pattern of the noise and information being separated into high and low frequencies Fourier coefficients, respectively, this process produces a denoised version of the spectrum.

Fourier denoising is fundamentally different from and inherently more powerful than working exclusively in direct space where common smooths like the Savitzky-Golay[2] and boxcar smooths are applied. Theoretically speaking, in a Savitzky-Golay smooth, one sequentially fits short segments of a spectrum to a polynomial, replacing the central point of the data segment with the polynomial fit to the group of data points around it. In a boxcar smooth, one averages a central data point in a data set with those around it, replacing the central data point with the average of the points. For obvious reasons, the number of data points smoothed at each step in these processes is almost always odd. To smooth a spectrum, this process is repeated sequentially for all the data points in it, except perhaps at the ends of the data set, where the points may need to be treated differently. In practice, both the Savitzky-Golay and boxcar smooths are performed by sequentially multiplying small groups of adjacent data points in direct space by a set of numbers, a kernel, and then summing these results for a given data point. Because, as noted, this process is repeated across the dataset, it is a discrete convolution.

While the Savitzky-Golay and boxcar smooths do remove noise from data, there are rather significant problems associated with using them.[1] Working only in direct space, it is difficult to select the right lengths for these smooths so that the Fourier transforms of the kernels of these smooths, i.e., their corresponding transfer functions, will be about unity at low frequencies and transition to zero at the higher frequencies where the noise first appears. Consequently, noise is often left in the data. In addition, the transfer functions of the Savitzky-Golay and boxcar smooths do not monotonically approach zero at higher frequencies. Rather, they tend to bounce. Accordingly, they leave high frequency noise in data. While adequate for some applications, they are, mathematically speaking, naïve approaches for removing noise.

In this tutorial, we first provide a general overview of Fourier analysis. This short section should provide the reader with enough information to use Fourier analysis to denoise many spectra at a reasonable level. We then go into detail mathematically about the Fourier transform, which is applied to continuous functions, and the discrete Fourier transform, which is applied to discrete sequences of data points. We discuss the Fourier transform of continuous functions first because it provides an important theoretical framework for understanding Fourier theory, including the discrete Fourier transform. Ironically, although the Fourier transform of continuous functions is an integral transform and the discrete Fourier transform is based on summations, people often struggle more to understand the summations in the discrete Fourier transform. Ultimately, the purpose of this article is to provide an understandable explanation of these mathematical tools such that the reader will ultimately have a solid foundation from which to use Fourier analysis to denoise data.

Here are some disclaimers/explanations associated with this article. First, while it is fairly long, it is not possible to cover every aspect of Fourier analysis in it. Thus, in comparison to any reasonable book on Fourier analysis, this work is incomplete. Second, we have tried to be more explicit in writing out many of the derivations and solutions to problems than is done in some other books on this topic. Our purpose in doing this is to make this document, and therefore Fourier theory, as accessible as possible to newcomers in the field. Finally, because we are interested in real data (spectra), we primarily deal with the Fourier transforms and discrete Fourier transforms of real, not imaginary, functions. Of course, the Fourier transforms and discrete Fourier transforms we get of functions and real data are, in general, complex.

Many books and related documents have been written on Fourier analysis, which complement and complete the information here.[3, 4, 6-18]

In addition, this work follows previous analyses of XPS data, including efforts to denoise it with wavelets,[19-22] and also analyses of whole spectra as vectors (in hyperspaces) using techniques that include principal component analysis (PCA),[23-25] multivariate curve resolution (MCR),[26] and cluster analysis.[27]

V. A QUICK GUIDE TO FOURIER THEORY: A PRACTICAL PERSPECTIVE ON DENOISING DATA

This section contains a brief introduction to the Fourier transform and discrete Fourier transform (DFT) and explains how the DFT can be used to denoise data. Although most of the information in this section, including the definitions of the Fourier transform and discrete Fourier transform and the ideas in the figures, will be repeated in the next sections, we think it is still a good idea to read this section before proceeding to the more mathematical part of this document. It provides a useful perspective on denoising data.

The Fourier transform is all about sinusoids. It works under the premise that reasonable, continuous functions can be decomposed into a set of underlying sines and cosines. For example, the function shown with the solid purple line in Figure 1 is composed of two sines and a cosine, which, parenthetically, were added together previously to make it. Both the frequencies and amplitudes of these underlying waves matter.

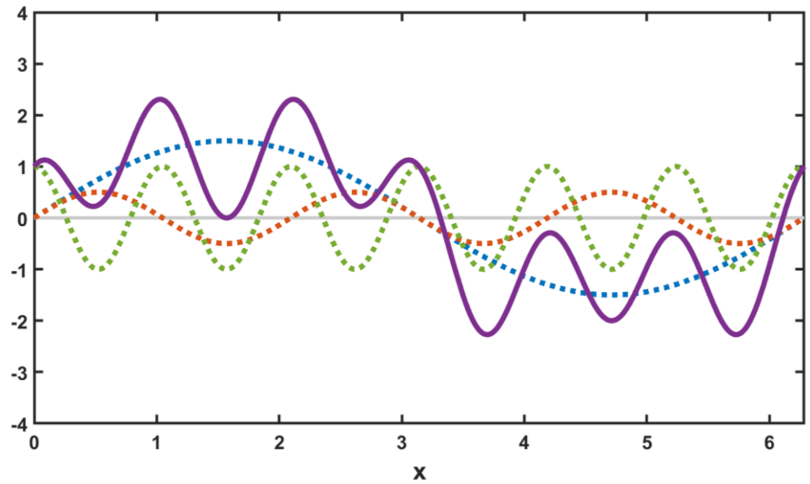

Figure 1. A function (solid purple line) created by summing a 'blue' sinusoid: 1.5 sin(x), an 'orange' sinusoid: 0.5 sin(3x), and a 'green' sinusoid: cos(6x).

The Fourier transform is commonly defined as follows:

$$F(s) = \int_{-\infty}^{\infty} f(x) e^{-i2\pi sx} dx \tag{1}$$

and the inverse Fourier transform as:

$$f(x) = \int_{-\infty}^{\infty} F(s) e^{i2\pi sx} ds. \tag{2}$$

That is, Equation 1 takes a function, $f(x)$, and transforms it into another function, $F(s)$. Note that x and s play different roles on the different sides of Equations 1 and 2. In Equation 1, s functions as a variable on the left side of the equation and as a constant on the other. In Equation 2, x functions as a variable on the left side of the equation and as a constant on the other.

Sometimes, to simplify the notation, the Fourier transform is represented as the operator: $\mathcal{F}$. That is, we might write Equation 1, where we increasingly simplify the notation here: $\mathcal{F}\{f(x)\} = \mathcal{F}f(x) = \mathcal{F}f = F(s) = F$, i.e., $\mathcal{F}f = F$. Similarly, one might write $\mathcal{F}^{-1}F = f$.

The Fourier transform and the inverse Fourier transform are not quite equivalent. They differ by a minus sign in the exponents of their kernels. That is, in Equation 1, the kernel is $e^{-i2\pi sx}$, and in Equation 2, the kernel is $e^{i2\pi sx}$. Thus, in general, taking the Fourier transform twice of a function does not quite return the original function. In other words, in general, $\mathcal{F}\mathcal{F}f \neq f$, although, as explained below, $\mathcal{F}\mathcal{F}f = f$ in an important special case.

The sinusoidal nature of the Fourier transform is revealed in Euler's relationship for complex exponentials:

$$e^{ix} = \cos(x) + isin(x) \tag{3}$$

Thus, for Equations 1 and 2 we can write:

$$e^{-i2\pi sx} = \cos(2\pi sx) - isin(2\pi sx) \tag{4}$$

and

$$e^{i2\pi sx} = \cos(2\pi sx) + isin(2\pi sx) \tag{5}$$

In Equation 1, s is the frequency of the sines and cosines that $f(x)$ is multiplied by. Indeed, we see in Equations 1 and 4 that $f(x)$ is multiplied by sines and cosines of every possible frequency, s, where the result (integral) for one value of s on the right side of Equation 1 gives the corresponding value of $F(s)$ for that particular value of s. Note that we also include negative values for s. Of course, negative frequencies don't exist in real life. Rather, they are a mathematical convenience here. In other words, at least theoretically, we need to perform an integral for each value of s.

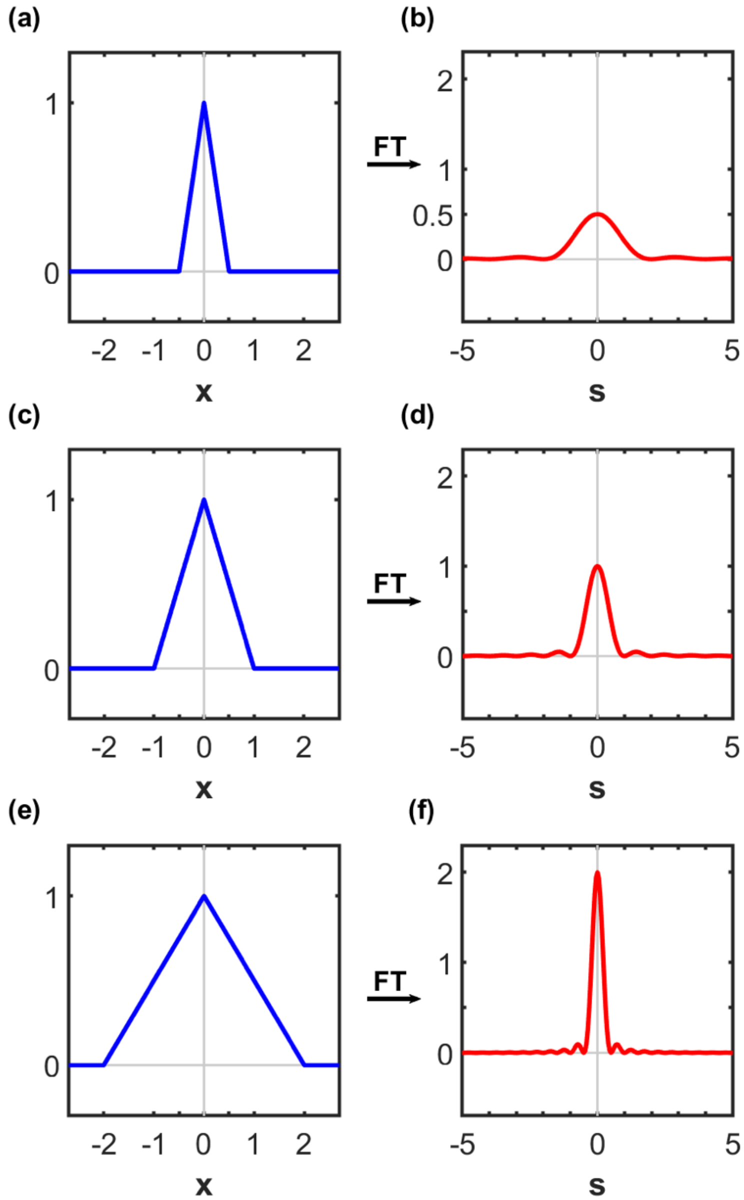

Figure 2. (a, c, and e) Three triangle functions with different widths and (b, d, and f) their respective Fourier transforms.

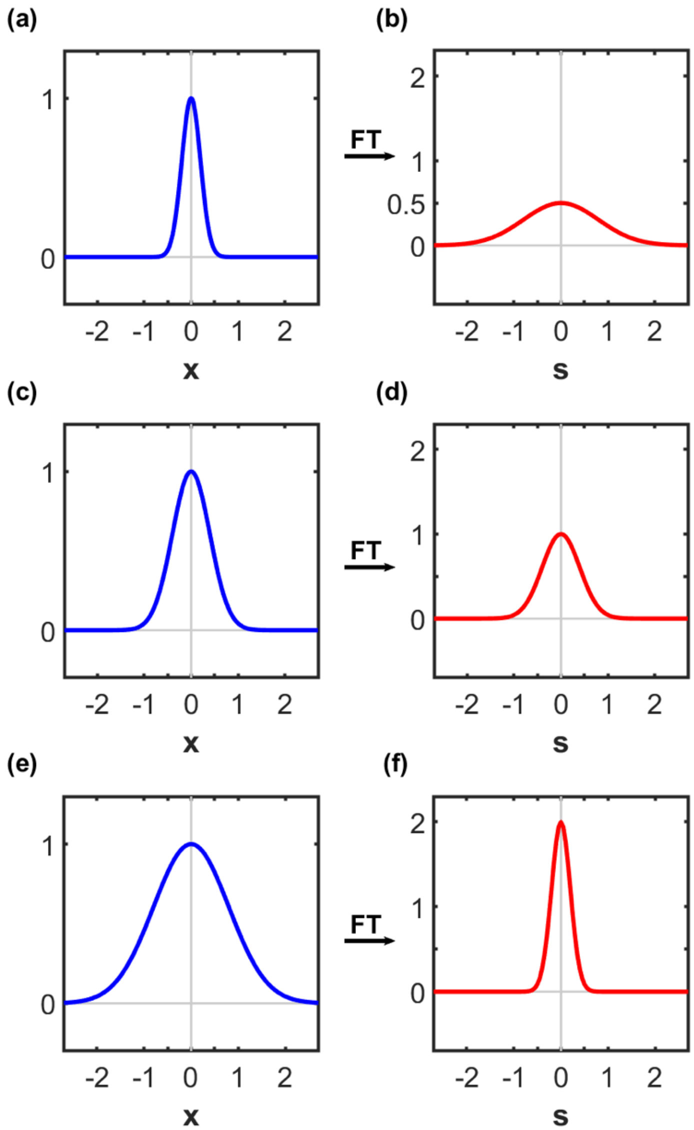

Figure 3. (a, c, and e) Three Gaussian functions with different widths and (b, d, and f) their respective Fourier transforms.

The Fourier transform has an important reciprocal property. Broader functions have narrower Fourier transforms, and narrower functions, or functions with sharp features, have broader Fourier transforms. In other words, broader functions are made up of fewer frequency components, and it takes a lot of frequency components to recreate narrow functions or sharp features. For example, Figure 2 shows three triangle functions that range from broader to narrower. Note that the Fourier transforms of these functions range oppositely from narrower to broader. Similarly, Figure 3 shows three Gaussian functions with different widths and their Fourier transforms. Again, the broader Gaussians have narrower Fourier transforms, and vice versa.

When the Fourier transform takes a function of interest, $f(x)$, and creates another function with a different variable, $F(s)$, from it, it also creates a new space or domain for $F(s)$. We refer to a function, $f(x)$, as being in direct space and its Fourier transform, $F(s)$, as being in indirect or reciprocal space. The word 'reciprocal' makes sense when we look at the units of x and s in $e^{-i2\pi sx}$ and $e^{i2\pi sx}$. They must cancel, i.e., x and s must have reciprocal units. For example, if x has units of time, s must have units of $^{1}/_{time}$ or frequency.

Both the theory of Fourier transforms and that of the discrete Fourier transform (DFT) are governed by a series of theorems. While not always essential for solving problems in Fourier analysis, these theorems often make problems much simpler. For data smoothing, the most important of these theorems is the convolution theorem. A convolution is the result of two functions acting on each other. In a convolution, one function is reversed and then shifted to every possible position relative to the other function. At each shift, the functions are multiplied together and integrated. The value of this integral is the value of the convolution at a particular shift. The concept of convolution shows up all over science. For example, a convolution takes place when a beam of white light that has been dispersed into its underlying colors, perhaps by a diffraction grating in a monochromator, is passed across a slit. A convolution is also taking place when the size of an X-ray beam in XPS is determined by passing it across a sharp interface.[28]

Convolution can be computationally expensive. It can require many multiplications. The convolution theorem simplifies this problem. It reveals that convolution in one domain is equivalent to multiplication in the other. Mathematically, the convolution of two functions, $f(x)$ and $g(x)$, is represented as $f(x) * g(x)$, where we will now assume that the Fourier transforms of $f(x)$ and $g(x)$ are $F(s)$ and $G(s)$, respectively. The convolution theorem tells us that $\mathcal{F}\{f(x) * g(x)\} = F(s)G(s)$. That is, convolution in one domain is equivalent to multiplication in the other! Thus, a computationally expensive convolution in direct space can be replaced with a multiplication of two functions in reciprocal space.

Ultimately, there are two problems with the Fourier transform, which is mostly used for continuous functions. First, the data we collect in real life are almost always discrete. For example, most spectra are collected at points (specific energies) that are regularly spaced in energy. Second, the Fourier integral in Equation 1 is hard to do even for moderately complex functions. Nevertheless, we would love to be able to apply the ideas and power behind the Fourier transform to real data to reveal the frequency content of the data. Fortunately, there is a way to do this through the discrete Fourier transform (DFT), which works on discrete data. The key ideas of the Fourier transform carry over into the DFT.

Convolution is also commonly practiced with discrete data. The act of smoothing data with, say, a simple boxcar function is a convolution. For example, in a five-point boxcar smooth, in each group of five adjacent points in a data set, each data point is multiplied by ${}^{1}/_{5}$ and the middle data point is replaced with the sum of these scaled data points.

There is also a convolution theorem for discrete data, which, as expected, offers computational advantages. Nevertheless, there are additional advantages to working in reciprocal space that are at least as great as the advantage of greater computational speed. The reciprocal space representation of a spectrum, e.g., of a typical XPS narrow scan, naturally divides it into a set of lower-index Fourier coefficients that describe the underlying signal and a set of higher-index

Fourier coefficients that describe the noise on the signal. Through the convolution theorem, one is able to multiply these Fourier coefficients by a transfer or filter function that largely removes the noise-containing, higher frequency Fourier coefficients while leaving the signal-containing lower frequency Fourier coefficients intact. After this multiplication in reciprocal space, the inverse Fourier transform of this product yields a denoised version of the spectrum. As we pointed out in a previous paper,[1] this approach is better than the traditional Savitzky-Golay[2] and boxcar smooths, which work in direct space. With these conventional smooths, it is difficult to know how long to make them (over how many data points) so that they will remove as much noise as possible from the data. Furthermore, these smooths do not decrease monotonically to zero in reciprocal space (they generally bounce around), which means that they leave high-frequency noise in the data. They are, at best, imperfect approaches to noise removal.

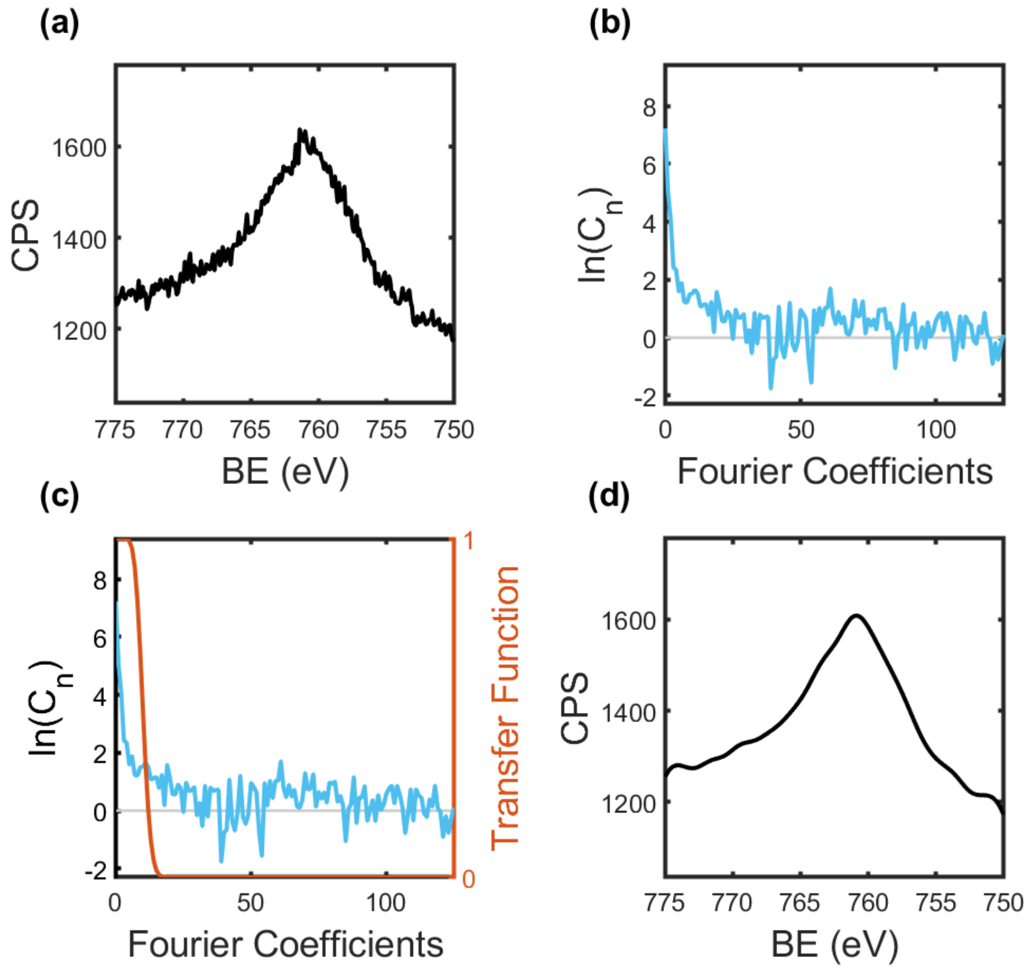

Figure 4. (a) An XPS narrow scan in direct space. (b) The DFT of the narrow scan in (a). (c) A Gauss-Hermite transfer function (orange) positioned on the DFT in (b). (d) The result of back transforming the product of the DFT and transfer function in (c).

Figure 4 reveals the process of denoising an XPS spectrum via the DFT and convolution theorem. That is, Figure 4a shows a moderately noisy XPS spectrum, and Figure 4b shows its Fourier coefficients (discrete Fourier transform). As indicated in the figure, the lower-index Fourier coefficients describe the underlying signal in the spectrum, and the higher-index Fourier coefficients describe the noise in it. Note that Figure 4a and Figure 4b are plotted on log scales. Figure 4c shows the so-called Gauss-Hermite transfer function,[29-31] which is sigmoidal (S-shaped), placed over the Fourier coefficients. As would be hoped for, this transfer function has a value of nearly unity for the lower-index Fourier coefficients and is nearly zero for higher-index Fourier coefficients. Furthermore, it is adjustable. Its cutoff can be positioned by the user so that it removes as much noise as possible from the data. In general, it should be placed near the inflection point or 'knee' in the data between the meaningful low-frequency Fourier coefficients and the noise-containing high-frequency Fourier coefficients. Small deviations from what might be considered optimal positioning for the transfer function usually do not affect the results of the smoothing very much. Finally, Figure 4d shows the result of back Fourier transforming the product of the Fourier transform of the spectrum and the transfer function in Figure 4c. A denoised version of the spectrum is produced.

The general approach for denoising data that is outlined here is used in the Fourier denoising of data. Accordingly, this section should provide the user with enough information to apply Fourier theory to many denoising problems. Greater detail regarding the theory behind the Fourier transform and discrete Fourier transform are now given below.

VI. The Fourier Transform

A. *Definitions of the Fourier transform*

1. *Definitions of the forward and inverse Fourier transforms we will use*

The Fourier transform of a continuous function $f(x)$ can be defined as:

$$F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx}dx \tag{6}$$

This integral transform takes a function of x, $f(x)$, and transforms it into a function of a different variable s, $F(s)$. Interestingly, s plays different roles on the two sides of Equation 6. It acts like a variable on the left side of Equation 6, but as a constant in the integral on the right side of it. We will see this pattern repeated in other areas of Fourier analysis, e.g., in convolution. The imaginary number i appears in the exponent of Equation 6 and similarly in many of the equations in this document, where $i = \sqrt{-1}$. Electrical engineers prefer to use $j = \sqrt{-1}$ to avoid confusing the symbol i as it is used mathematically with their symbol for current, which is also i. As Blanchard, Devaney, and Hall put it hilariously in their book on differential equations, "Electrical engineers use the symbol i for current because current starts with c."[32] The Fourier transform can be represented as an operator, $\mathcal{F}$, acting on a function, which is a more compact notation. Thus, Equation 6 may be rewritten with increasing degrees of brevity as:

$$F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx}dx = \mathcal{F}\{f(x)\} = \mathcal{F}f(x) = \mathcal{F}f \tag{7}$$

Equation 6 implies that there must be a relationship between the units of x and s because the product sx in $e^{-i2\pi sx}$ must be dimensionless. Hence, so that they will cancel, x and s must have reciprocal units. For example, we can rewrite Equation 6 in terms of time, t, and frequency, f, which has units of $1/time$, as follows:

$$F(f) = \int_{-\infty}^{\infty} f(t)e^{-i2\pi ft}dt \tag{8}$$

Unfortunately, the inverse, or reverse, or back Fourier transform is not quite the same as the forward Fourier transform in Equation 6, although they are quite similar. They differ by a minus sign in their kernels, i.e., in $e^{-i2\pi sx}$ vs. $e^{i2\pi sx}$. That is, the inverse Fourier transform for continuous functions is:

$$f(x) = \int_{-\infty}^{\infty} F(s)e^{i2\pi sx}ds. \tag{9}$$

Similar to what we observed in Equation 6, and as would be expected, x acts as a variable on the left side of Equation 9 and as a constant in the integral on the right side of Equation 9. In addition, as is suggested in Equation 7, we can use the operator, $\mathcal{F}^{-1}$, to represent the inverse Fourier transform as follows:

$$f(x) = \int_{-\infty}^{\infty} F(s)e^{i2\pi sx}ds = \mathcal{F}^{-1}\{F(s)\} = \mathcal{F}^{-1}F = f \tag{10}$$

2. Other definitions of the Fourier transform, and why the definition in this work was chosen

Unfortunately, Equations 6 and 9 are not the only definitions of the forward and inverse Fourier transforms. There are others, which differ in the locations of the '2π' term in the equations. While these different definitions do not, in general, significantly change the results obtained by Fourier transforming a function, some of the detail in the answers obtained with them is usually different. The situation is actually rather humorous. Different authors have different preferences, where a few authors are quite insistent on the equations they prefer. One author went so far as to warn readers not to listen to anyone who might suggest that they use any equations except the ones he prefers. Authors like this sort of imply that those who do not use their preferred equations are morons. Equations 6 and 9 are used extensively by Bracewell, who advocated for them.[3] These equations have several virtues. They (i) make a number of Fourier transforms, including some of the important Fourier transform pairs that will be discussed below, turn out very nicely/simply, where these pairs are usually a little more complicated when the other definitions of the Fourier transform are employed, (ii) put the '2π' term in the same place in the forward and back transforms (in the exponent of the exponential), where some of the other definitions of the Fourier transform are sometimes not quite as symmetric, so it is arguably easier to remember Equations 6 and 9, (iii) put the '2π' term in the same place in the forward and back Fourier transforms as they appear in the discrete Fourier transform (in the exponentials), (iv) create a clear meaning for x and s and t and f in Equations 6 and 8, respectively, e.g., in Equation 8, f is the number of cycles $cos(2\pi ft)$ and $sin(2\pi ft)$ have undergone when $t = 1$ (if this doesn't make sense to you, see the section below on Euler's relationship), (v) are widely, but not exclusively, used, and (vi) are well accepted. Accordingly, Equations 6 and 9 will be used in this work.

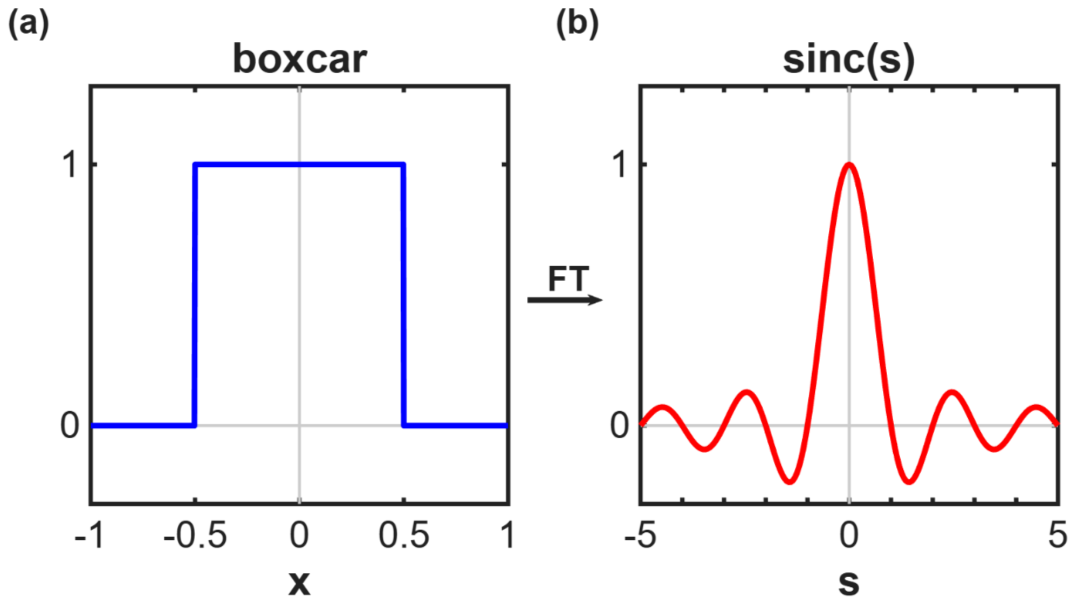

Figure 5. (a) The boxcar function, as defined in Equation 11, and its Fourier transform (b) the $sinc(s)$ function.

3. A simple, but relevant, example of calculating a Fourier transform

We now calculate the Fourier transform of the so-called boxcar or top hat function, which can be defined as:

$$\Pi(x) = \begin{cases} 1, & |x| \leq \frac{1}{2} \\ 0, & |x| > \frac{1}{2} \end{cases} \tag{11}$$

This function is shown in Figure 5a, where the capital Greek letter pi, $\Pi(x)$, is sometimes used for this function because it resembles the shape of the function. However, before moving on, note that the boxcar function could just as easily have been defined as:

$$\Pi_a(x) = \begin{cases} 1, & |x| < \frac{1}{2} \\ 0, & |x| \geq \frac{1}{2} \end{cases} \tag{12}$$

where $\Pi(x)$ and $\Pi_a(x)$ differ in how they are defined at $x = \pm\frac{1}{2}$. As we will see, this slight difference will not make any difference in their Fourier transforms. Equations 11 and 12 have the same Fourier transform.

To calculate the Fourier transform of $\Pi(x)$, we insert $\Pi(x)$ into Equation 6, which, according to its definition, is unity from $-\frac{1}{2}$ to $+\frac{1}{2}$ and zero otherwise. This leads us to:

$$F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx}dx = \int_{-\infty}^{\infty} \Pi(x)e^{-i2\pi sx}dx \tag{13}$$

$$= \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{-i2\pi sx}dx = \frac{-1}{i2\pi s}e^{-i2\pi sx}\Big|_{-\frac{1}{2}}^{\frac{1}{2}} = \frac{i}{2\pi s}\left(e^{-i\pi s} - e^{i\pi s}\right)$$

$$= \frac{i}{2\pi s}\big(\cos(\pi s) - isin(\pi s) - \cos(\pi s) - isin(\pi s)\big) = \frac{sin(\pi s)}{\pi s}$$

$$= sinc(s)$$

where, again, Euler's relationship was used here (see again explanation below if you are not familiar with it). The $\frac{sin(\pi s)}{\pi s}$, or $sinc(s)$ function (see Figure 5b), is important in Fourier theory, which is one of the reasons why it has its own name. Thus, we say that $\Pi(x)$ and $sinc(s)$ are a Fourier transform pair, which we can represent as $\Pi(x) \leftrightarrow sinc(s)$. We will encounter other interesting pairs below.

Two final notes. First, while $sinc(0) = \frac{sin(\pi 0)}{\pi 0} = \frac{0}{0}$, L'Hôpital's rule reveals that $sinc(0) = 1$. Second, the $sinc$ function is also sometimes defined such that $sinc(s) = \frac{sin(s)}{s}$.

4. An aside on null functions

This section explains why $\Pi(x)$ (Equation 11) and $\Pi_a(x)$ (Equation 12) have the same Fourier transforms.

For years, Linford has played tennis both with a variety of opponents and on United States Tennis Association (USTA) league teams. He plays a few times a week. Unfortunately, he doesn't win all his matches, and lately it seems like he's been losing a rather large fraction of his matches. While these losses always hurt, and may even ruin his day, he tries to remind himself that, at the end of the day, league tennis is all about nothing, which, by the way, is a good reason to keep your cool and not smash the ball, scream, throw your racket, and swear when you miss a shot, even an important shot. Most people appreciate a gracious loser.

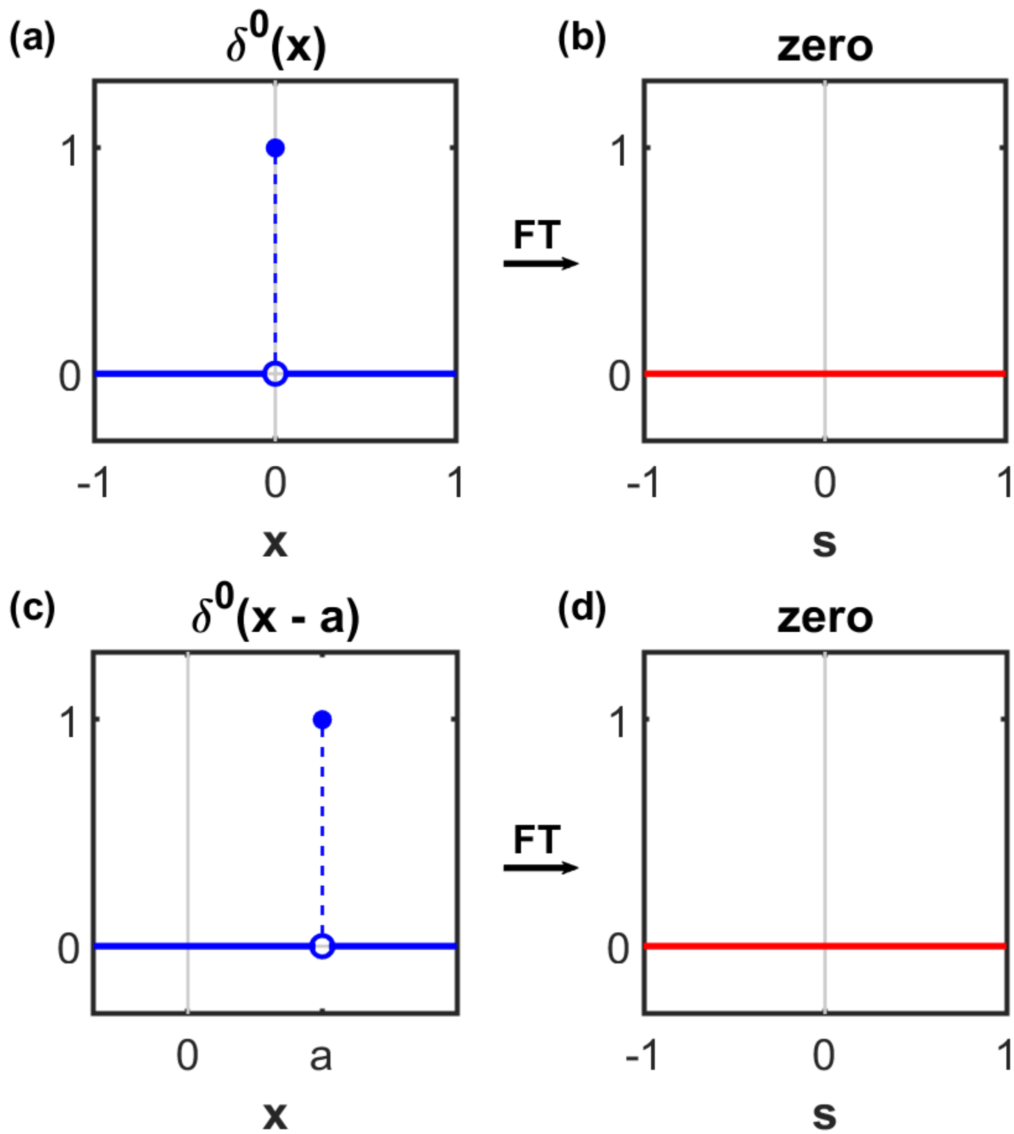

Figure 6. (a) Representation of the null function, $\delta^0(x)$, defined in Equation 15 and (b) its Fourier transform, which is zero. (c) Representation of the null function $\delta^0(x-a)$, as defined in the text, and (d) its Fourier transform, which is zero.

Null functions are also all about nothing. Null functions have integrals of zero even though they themselves are not zero. $N(x)$ is a null function if:

$$\int_{-\infty}^{\infty} |N(x)| dx = 0 \tag{14}$$

For example, Bracewell[3] defines the null function $\delta^0(x)$, which is nonzero at just a single point (see Figure 6a), as follows:

$$\delta^0(x) = \begin{cases} 0, & x \neq 0 \\ 1, & x = 0 \end{cases} \tag{15}$$

The null function is a strange function. After Linford explained null functions to one of his colleagues, the colleague remarked: “They don’t sound like they’re very useful”. As we will see, there are other strange functions in Fourier theory.

Obviously, we could shift the null function in Equation 15 to another position, say a, on the x-axis, which we would represent as $\delta^0(x-a)$. Figure 6c shows a plot of $\delta^0(x-a)$.

The null function gives us a precise way (down to the last point) to think about definitions of functions. For example, we might define another boxcar function, $\Pi_b(x)$, that does not even define the function at $x = \pm\frac{1}{2}$.

$$\Pi_b(x) = \begin{cases} 1, & |x| < \dfrac{1}{2} \\ 0, & |x| > \dfrac{1}{2} \end{cases} \tag{16}$$

We could then relate $\Pi(x)$ to $\Pi_b(x)$, as follows: $\Pi(x) = \Pi_b(x) + \delta^0\left(x - \frac{1}{2}\right) + \delta^0\left(x + \frac{1}{2}\right)$.

As might be expected, the Fourier transform of a null function is zero (see Figure 6b and d), where we will provide a theoretical justification for this statement below. Thus:

$$\int_{-\infty}^{\infty} \delta^0(x) e^{-i2\pi sx} dx = 0 \tag{17}$$

From Equation 17, we can see mathematically why $\Pi(x)$, $\Pi_a(x)$, and $\Pi_b(x)$ all have the same Fourier transform. For example:

$$\begin{aligned}
&\int_{-\infty}^{\infty} \Pi(x) e^{-i2\pi sx} dx \\
&= \int_{-\infty}^{\infty} (\Pi_b(x) + \delta^0\left(x - \frac{1}{2}\right) + \delta^0\left(x + \frac{1}{2}\right)) e^{-i2\pi sx} dx \\
&= \int_{-\infty}^{\infty} \Pi_b(x) e^{-i2\pi sx} dx \\
&+ \int_{-\infty}^{\infty} \delta^0\left(x - \frac{1}{2}\right) e^{-i2\pi sx} dx \\
&+ \int_{-\infty}^{\infty} \delta^0\left(x + \frac{1}{2}\right) e^{-i2\pi sx} dx = \int_{-\infty}^{\infty} \Pi_b(x) e^{-i2\pi sx} dx
\end{aligned} \tag{18}$$

The theory behind what we just discussed is described in Lerch's theorem,[3] which states that if two function, e.g., $f_1(x)$ and $f_2(x)$, have the same Fourier transform, then the difference between them, $f_1(x) - f_2(x)$, is a null function. So, two functions that have the same Fourier transform are not necessarily identical.

B. *Euler's formula: Fourier analysis is about sinusoids, and roots of unity*

1. Euler's formula

Central to the Fourier transform and inverse Fourier transform are their $e^{-i2\pi ft}$ and $e^{i2\pi sx}$ terms (kernels), respectively. These can be expanded with Euler's relationship, which is:

$$e^{ix} = cos(x) + isin(x) \tag{19}$$

and similarly:

$$e^{-ix} = cos(x) - isin(x) \tag{20}$$

Euler's formula often appears mysterious to those who have not seen it before. Nevertheless, it is easily proved by adding the Taylor series expansions of e^{ix}, $cos(x)$, and $i\ sin(x)$, which is left for the reader to do. Using Euler's relationship, we can rewrite Equation 6 as:

$$\begin{aligned} F(s) &= \int_{-\infty}^{\infty} f(x)\,(cos(2\pi sx) - isin(2\pi sx))\,dx \\ &= \int_{-\infty}^{\infty} f(x)\,cos(2\pi sx)dx - i\int_{-\infty}^{\infty} f(x)\,sin(2\pi sx)\,dx \end{aligned} \tag{21}$$

and Equation 9 as:

$$f(x) = \int_{-\infty}^{\infty} F(s)\,(cos(2\pi sx) + isin(2\pi sx))\,ds \tag{22}$$

$$= \int_{-\infty}^{\infty} F(s)\,cos(2\pi sx)ds + i\int_{-\infty}^{\infty} F(s)\,sin(2\pi sx)\,ds$$

Euler's relationship reveals that there are, in general, real and imaginary parts to the forward and inverse Fourier transforms. Accordingly, even though spectra are usually real functions, their Fourier transforms generally have both real and imaginary parts. Equations 19 – 22 reveal that the Fourier transform is very much about sinusoids. Furthermore, while not done in this article, we can start with a complex function and Fourier transform it, which, in general, will produce another complex function.

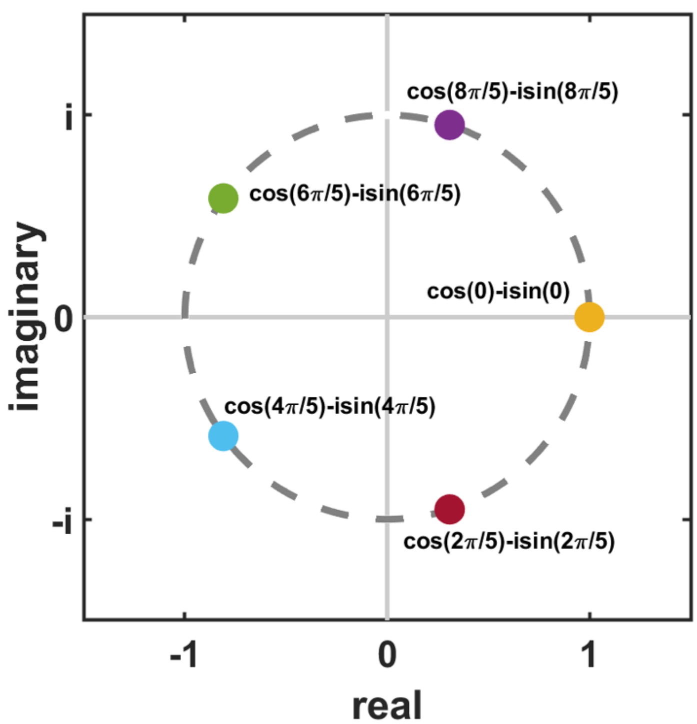

Figure 7. The five unique roots of unity for $e^{-i2\pi n/5}$.

As an illustration of the use of imaginary numbers in exponents and Euler's formula, Equation 19, we consider the idea of the roots of unity. Of course, we appreciate that $1^2 = 1$ and $(-1)^2 = 1$, and with our understanding of i we now see that $i^4 = 1$, so 1, -1, and i are roots of unity. Are there other situations like this? Is there a number x other than one such that $x^5 = 1$ or $x^{127} = 1$? The simple answer is yes. We can construct such numbers from Euler's relationship, where we first recognize that:

$$e^{\pm i2\pi} = cos(2\pi) \pm isin(2\pi) = cos(2\pi) = 1, \qquad (23)$$

and in addition, for n an integer:

$$e^{\pm i2\pi n} = cos(2\pi n) \pm isin(2\pi n) = cos(2\pi n) = 1 \qquad (24)$$

To illustrate these concepts, let's now consider the properties of $e^{\pm i2\pi n/5}$ and $e^{\pm i2\pi n/127}$, where, again n is an integer. We see that $\left(e^{\pm i2\pi n/5}\right)^5 = 1$ and $\left(e^{\pm i2\pi n/127}\right)^{127} = 1$, so $e^{\pm i2\pi n/5}$ and $e^{\pm i2\pi n/127}$ are roots of unity. Furthermore, note that $e^{\pm i2\pi n/5}$ and $e^{\pm i2\pi n/127}$ are roots of unity for any values of n, which, again, is an integer. Exploring this further, let's consider $n + 5$ in $e^{-i2\pi n/5}$, which will give us $e^{-i2\pi(n+5)/5} = e^{-i2\pi n/5}e^{-i2\pi} = e^{-i2\pi n/5}$. Thus, $e^{-i2\pi n/5}$ has a period of 5 so $e^{-i2\pi n/5}$ shows unique roots of unity for $n = 0, 1, 2, 3, 4$, where, due to the periodicity, we get the same answer for $n = 0$ and $n = 5$, $n = 1$ and $n = 6$, etc.

Finally, we should not overlook the important graphical interpretation of $e^{-i2\pi n/5}$, which is that these roots of unity lie on a unit circle in the complex plane. For example, from Euler's relationship, $n = 0, 1, 2, 3, 4$ in $e^{-i2\pi n/5}$ give us:

$$e^{-i2\pi 0/5} = cos(0) - isin(0) = 1 \tag{25}$$

$$e^{-i2\pi 1/5} = cos(2\pi/5) - isin(2\pi/5) \tag{26}$$

$$e^{-i2\pi 2/5} = cos(4\pi/5) - isin(4\pi/5) \tag{27}$$

$$e^{-i2\pi 3/5} = cos(6\pi/5) - isin(6\pi/5) \tag{28}$$

$$e^{-i2\pi 4/5} = cos(8\pi/5) - isin(8\pi/5) \tag{29}$$

Figure 7 shows a plot of the results in Equations 25 –29, which do indeed lie on the unit circle in the complex plane. Again, increasing the value of n beyond 4 produces the same values on the unit circle.

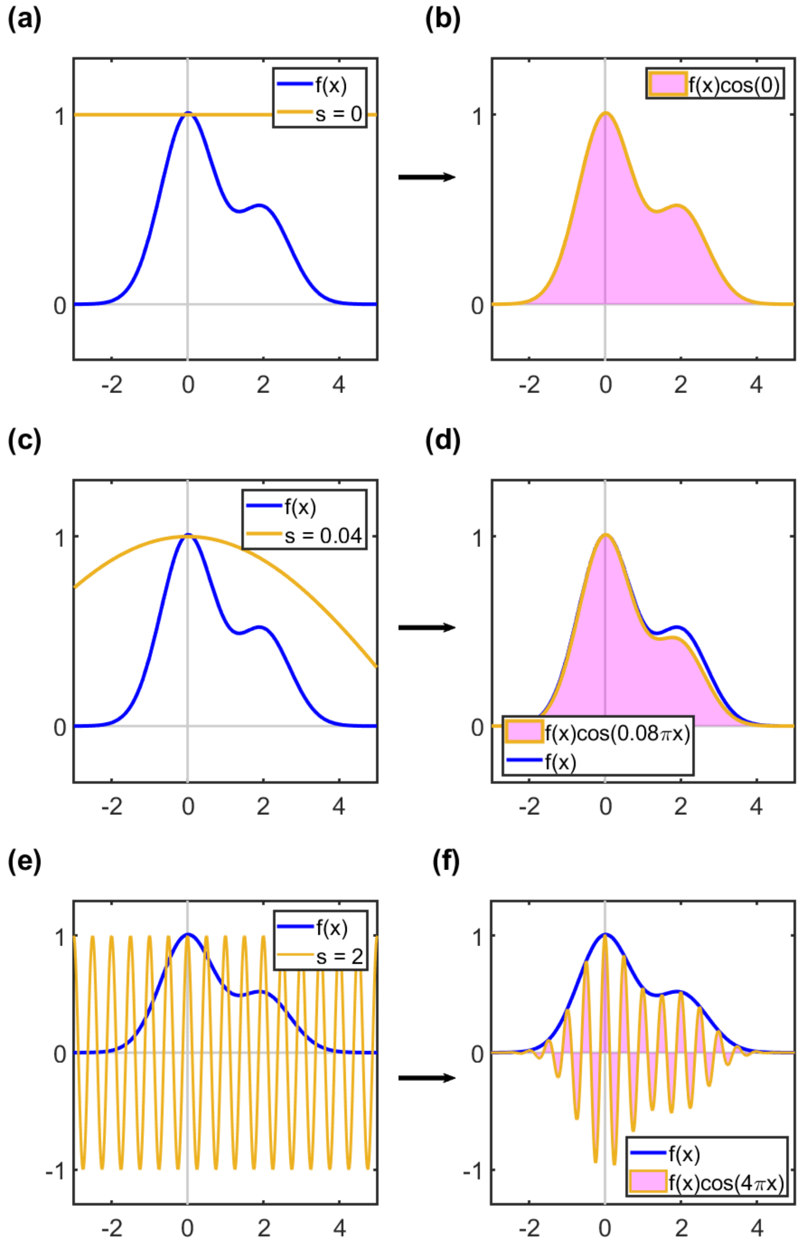

Figure 8. Graphical illustration of the Fourier transform of an arbitrary function, $f(x)$, for different values of s in $F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx}dx$ showing that (a – b) $F(0) = \int_{-\infty}^{\infty} f(x)dx$ and (c – f) suggesting that if $f(x)$ has finite support (it is only non-zero over a limited range of x values) $\lim_{s\to\infty} F(s) = 0$.

C. *Developing some graphical insight into the Fourier transform. The Fourier transform of a function with finite support as $s \to 0$ and $s \to \pm\infty$.*

To obtain a greater graphical sense for the Fourier transform, we take advantage of Euler's relationship (Equation 20) in Equation 6, which gives:

$$F(s) = \int_{-\infty}^{\infty} f(x)\cos(2\pi sx)dx - i\int_{-\infty}^{\infty} f(x)\,sin(2\pi sx)\,dx \tag{30}$$

We now consider an arbitrary function, $f(x)$, which is plotted in Figure 8. As previously taught, s acts like a variable on the left of Equation 30 and as a constant on its right side. In math, it is often helpful to consider functions in their limits as their variables or parameters go to extreme values. Accordingly, we first consider $s = 0$ in Equation 30, which gives:

$$F(0) = \int_{-\infty}^{\infty} f(x)\cos(0)dx - i\int_{-\infty}^{\infty} f(x)\,sin(0)\,dx = \int_{-\infty}^{\infty} f(x)dx \tag{31}$$

In other words, at $s = 0$, which is the lowest frequency we can have for the cosine and sine terms, the Fourier transform of the function, $f(x)$, is just the area of the function (because we are multiplying it by unity) (see Figure 8a – b). Furthermore, at relatively small values of $|s|$, i.e., $|s| \approx 0$, $F(s)$ will, in general, also be close to the area of the function (see Figure 8c – d).

We now consider what happens to Equation 30 as $s \to \pm\infty$, where we rewrite it as:

$$\lim_{s\to\pm\infty} F(s) = \lim_{s\to\pm\infty} \int_{-\infty}^{\infty} f(x)\cos(2\pi sx)dx - i \lim_{s\to\pm\infty} \int_{-\infty}^{\infty} f(x)\, sin(2\pi sx)\, dx \tag{32}$$

We are assuming here that $f(x)$ has finite support, which means that $f(x)$ is non-zero only over a limited range of x values. As $s \to \pm\infty$ in $\cos(2\pi sx)$ and $\sin(2\pi sx)$ in Equation 32, these sinusoids oscillate with frequencies that approach infinity. Thus, when we evaluate Equation 32 for $f(x)$ and these sinusoids, the adjacent positive and negative parts of $f(x)\cos(2\pi sx)$ and $f(x)\, sin(2\pi sx)$, i.e., the adjacent parts of these functions in the negative and positive half-planes, will have nearly equal areas and will cancel, e.g., see $f(x)\cos(2\pi sx)$ in Figure 8e – f. This implies that for a continuous, well-behaved function with finite support $\lim_{s\to\pm\infty} F(s) = 0$.

D. *Even and odd functions*

Although most functions are neither even nor odd, the evenness and oddness of functions play an important role in Fourier analysis. Indeed, while it is, basically, a tautology to say this, it should be stated that all functions are either even, odd, or neither. In other words, and here is the tautology, functions either possess symmetry or they do not.

Even functions are symmetric with respect to the y-axis. The y-axis acts like a mirror for these functions, reflecting them back into themselves. We will refer to a generic even function as $E(x)$. Thus, even functions have the important property that $E(x) = E(-x)$. Examples of even functions include the cosine function, the function $f(x) = k$, where $k \in \mathbb{R}$, i.e., k is a real number, the function $f(x) = x^2$ (a simple parabola), unshifted Gaussian functions with the general form $f(x) = e^{-x^2}$, and unshifted Lorentzian functions with the general form $f(x) = \frac{1}{1+x^2}$.

Odd functions, which we will generically refer to as $O(x)$, also possess symmetry, but of a different kind. The origin acts as a center of inversion for odd functions. Thus, odd functions have the important property that $O(x) = -O(-x)$. Examples of odd functions include the sine function, the function $f(x) = kx$, where $k \in \mathbb{R}$, the function $f(x) = x^3$, and the function $f(x) = 1/x$ (a hyperbola).

The only function that is both even and odd is the zero function: $f(x) = 0$.

Examples of functions that are neither even nor odd are, in general, sums of even and odd functions like $f(x) = x^3 + 1$ and $f(x) = e^{-x^2} + x$. The functions e^{-x} and e^x are important examples of functions that are neither even nor odd. Most shifted sine and cosine functions are neither even nor odd.

As we will show below, we can unambiguously divide any real function, $f(x)$, into even and odd parts, where:

$$E(x) = \frac{1}{2}\big(f(x) + f(-x)\big) \tag{33}$$

and

$$O(x) = \frac{1}{2}\big(f(x) - f(-x)\big) \tag{34}$$

Thus, $f(x) = E(x) + O(x)$.

To show that the decomposition in Equations 33 and 34 is unique, imagine that we could decompose $f(x)$ into different even and odd functions, as follows:

$$f(x) = E_1(x) + O_1(x) \tag{35}$$

$$f(x) = E_2(x) + O_2(x) \tag{36}$$

where $E_1(x) \neq E_2(x)$ and $O_1(x) \neq O_2(x)$. Because they are both equal to $f(x)$, we can set Equations 35 and 36 equal to each other, which yields:

$$E_1(x) + O_1(x) = E_2(x) + O_2(x) \tag{37}$$

and with a little algebra we obtain:

$$E_1(x) - E_2(x) = O_2(x) - O_1(x) \tag{38}$$

However, as can be shown by the definition of even and odd functions, the sum or difference of two even functions is another even function, and the sum or difference of two odd functions is another odd function. Thus, in Equation 38 we have an even function, $E_1(x) - E_2(x)$, equal to an odd function, $O_2(x) - O_1(x)$. However, as noted above, the only function that is both even and odd is the zero function, which implies that:

$$E_1(x) - E_2(x) = O_2(x) - O_1(x) = 0 \tag{39}$$

Thus, $E_1(x) = E_2(x)$ and that $O_1(x) = O_2(x)$, which concludes our proof that the decomposition of a function into even and odd functions is unique.

E. *The Fourier transforms of even and odd functions*

The reader may wish to verify that the product, $E_{E_1E_2} = E_1E_2$, of two arbitrary even functions, E_1 and E_2, is another even function, the product, $E_{O_1O_2} = O_1O_2$, of two arbitrary odd functions, O_1 and O_2, is also an even function, and the product, $O_{E_1O_1} = E_1O_1$, of an arbitrary even function, E_1, and an arbitrary odd function, O_1, is an odd function. Also, recall from the previous section that the cosine function is even and the sine function is odd. In addition, from calculus we remember the following properties of even, $E(x)$, an odd, $O(x)$, functions in integrals, which follow directly from their symmetry:

$$\int_{-\infty}^{\infty} E(x)dx = 2\int_{0}^{\infty} E(x)dx \tag{40}$$

and

$$\int_{-\infty}^{\infty} O(x)dx = 0 \tag{41}$$

The Fourier transforms of even and odd functions have interesting properties that follow from the concepts we just reviewed. We first consider the Fourier transform of an even function, $E(x)$, in Equation 30, which becomes:

$$F_E(s) = \int_{-\infty}^{\infty} E(x)\cos(2\pi sx)dx - i\int_{-\infty}^{\infty} E(x)\, sin(2\pi sx)\, dx \tag{42}$$

The integrand of the first integral in Equation 42 is the product of two even functions, which is even, and the integrand of the second integral is the product of an even function and an odd function, which is odd. Thus, Equation 42 reduces to:

$$F_E(s) = 2\int_{0}^{\infty} E(x)\, cos(2\pi sx)dx \tag{43}$$

We next consider the Fourier transform of an odd function, $O(x)$. Thus, Equation 30 becomes:

$$F_O(s) = \int_{-\infty}^{\infty} O(x)\, cos(2\pi sx)dx - i\int_{-\infty}^{\infty} O(x)\, sin(2\pi sx)\, dx \tag{44}$$

Using the properties of even and odd functions we just discussed, this equation reduces to:

$$F_O(s) = -2i\int_{0}^{\infty} O(x)\, sin(2\pi sx)dx \tag{45}$$

There is a delightful subtlety in Equations 43 and 45 that should not go unnoticed. First, in simplifying Equations 42 and 44 to get Equations 43 and 45, respectively, we used the fact that $E(x)$, $O(x)$, $\cos(2\pi sx)$, and $\sin(2\pi sx)$ are treated as functions of x (not s) in their respective integrals, i.e., we integrated with respect to x. However, the question arises as to whether $F_E(s)$ and $F_O(s)$ from Equations 43 and 45 are themselves even or odd. Please note that $F_E(s)$ and $F_O(s)$ are functions of s, not x. Accordingly, to determine whether $F_E(s)$ is even or odd we consider $F_E(-s)$, which, from Equation 43, gives:

$$F_E(-s) = 2\int_0^\infty E(x)\,cos(-2\pi sx)dx = 2\int_0^\infty E(x)\,cos(2\pi sx)dx = F_E(s) \tag{46}$$

so $F_E(s)$ is even. Applying the same procedure for $F_O(s)$ in Equation 45, we obtain:

$$F_O(-s) = -2i\int_0^\infty O(x)\,sin(-2\pi sx)dx = 2i\int_0^\infty O(x)\,sin(2\pi sx)dx = -F_O(s) \tag{47}$$

so $F_O(s)$ is odd. That is, although the integrands of Equations 43 and 45 are even (if they were odd they would disappear), $F_E(s)$ is even and $F_O(s)$ is odd. An important conclusion here is that the Fourier transform of a real even function is a real even function, and the Fourier transform of a real odd function is an imaginary odd function.

We now consider the decomposition of a generic, real function into its even and odd parts: $f(x) = E(x) + O(x)$ and consider its Fourier transform. As noted, most functions are neither even nor odd, so this is the more general case for Fourier analysis. We now go back to the definition of the Fourier transform and consider the mathematics of this Fourier transform step by step.

$$F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx}dx \tag{48}$$

$$= \int_{-\infty}^{\infty} \big(E(x) + O(x)\big)e^{-i2\pi sx}dx$$

$$= \int_{-\infty}^{\infty} (E(x) + O(x))(cos(2\pi sx) - isin(2\pi sx))dx$$

Multiplying the terms in the last equation of Equation 48 gives:

$$\int_{-\infty}^{\infty} E(x)\cos(2\pi sx)\,dx - i\int_{-\infty}^{\infty} E(x)sin(2\pi sx)dx + \int_{-\infty}^{\infty} O(x)\cos(2\pi sx)\,dx \tag{49}$$

$$- i\int_{-\infty}^{\infty} O(x)sin(2\pi sx)dx$$

The middle two of these terms are zero because their integrands are odd, i.e., they are the products of even and odd functions, so Equation 49 reduces to:

$$\int_{-\infty}^{\infty} E(x)\cos(2\pi sx)\,dx - i\int_{-\infty}^{\infty} O(x)sin(2\pi sx)dx \tag{50}$$

As noted above, $\int_{-\infty}^{\infty} E(x)\cos(2\pi sx)\,dx$ is an even function and $\int_{-\infty}^{\infty} O(x)sin(2\pi sx)dx$ is an odd function. Hermitian functions are functions that have even parts that are real and odd parts that are imaginary. Thus, we have the important result that the Fourier transforms of real functions are Hermitian.

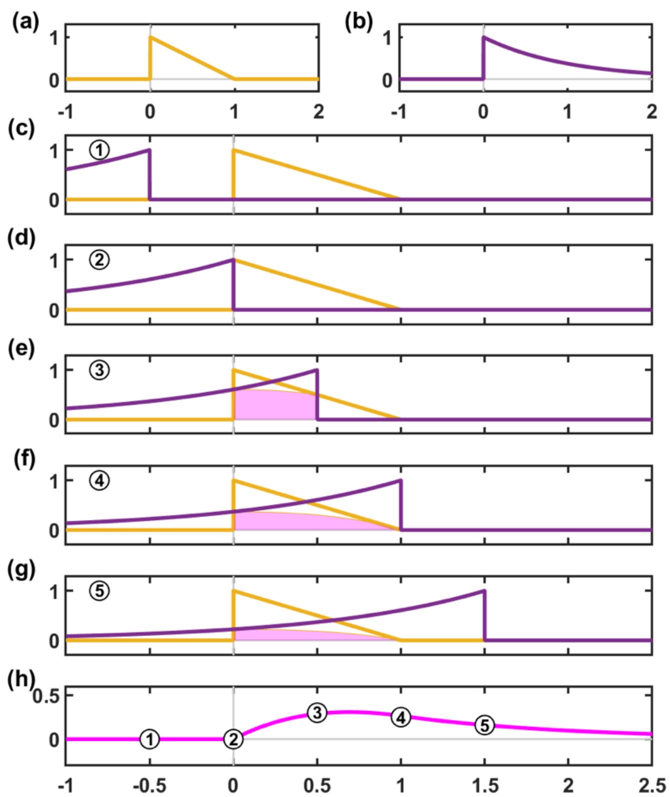

Figure 9. A graphical illustration of convolution. (a – b) Two functions to be convolved, where the triangular function is unchanged and the decaying exponential function will be reversed and shifted to various positions. (c – g) A graphical representation of the convolution between the functions in (a) and (b). (h) The convolution of the functions in (a) and (b) with the areas (pink) from the products of the functions in panels (c – g) noted.

F. *Convolution*

In preparation to prove the convolution theorem, which is the most important of the theorems discussed in this work for the denoising of data, we now explain convolution. As an aside, the traditional Savitzky-Golay and boxcar smooths mentioned above are employed as convolutions in direct space. Mathematically, the convolution of two functions, $f(x)$ and $g(x)$, which is indicated with the symbol $'*'$, is defined as:

$$h(x) = f(x) * g(x) = \int_{-\infty}^{\infty} f(\tau)\, g(x-\tau) d\tau \tag{51}$$

That is, when the functions we wish to convolve, $f(x)$ and $g(x)$, go into the convolution integral (Equation 51), we switch the variable x to a new variable, τ, which is a dummy variable. The variable we integrate over in a definite integral is called a dummy variable. Dummy variables 'disappear' at the end of an integration when the limits are applied. Accordingly, we can use whatever symbol we want for a dummy variable in a definite integral because it will also 'disappear'. However, we also have an entity, x, in this integral, which, as was the case for the Fourier integral, behaves as a variable on the left side of the equation, i.e., in $h(x)$, but as a constant in $\int_{-\infty}^{\infty} f(\tau)\, g(x-\tau) d\tau$, where x shifts the function $g(\tau)$. That is, in a convolution, one function, $f(x)$, remains unchanged and unshifted, while the other function, $g(x-\tau)$, is reversed because of the $'-\tau'$ part of it and then shifted to every possible position on the x-axis because of the $'x'$ part of it. At each shift, x, the functions $f(\tau)$ and $g(x-\tau)$ are multiplied together and integrated, which produces one value of $h(x)$. Thus, convolution in direct space, e.g., of discrete data, can require many computations. As we will see below, the convolution theorem provides a way around this issue. Figure 9 shows, graphically, an example of the convolution of two functions. Note that, in general, and as is illustrated in Figure 9, convolution broadens and smooths functions.

An important property of convolution is that it is commutative. That is:

$$f(x) * g(x) = g(x) * f(x) \tag{52}$$

As shown in Equation 53, this result can be proved in a few steps. First, in Equation 53, we change the variable in Equation 51 to $\tau' = x - \tau$, where, for this change of variables, $d\tau' = -d\tau$, which means that the limits of integration flip. In the next to last equation in Equation 53, the minus sign and the flipped integral limits reverse each other. At the same time, we replace τ' with τ because τ' is a dummy variable in the integral. By the definition of convolution, the next to last equation in Equation 53 is equal to $g(x) * f(x)$, which completes our proof.

$$\begin{aligned} h(x) = f(x) * g(x) &= \int_{-\infty}^{\infty} f(\tau)\, g(x-\tau) d\tau = \int_{\infty}^{-\infty} f(x-\tau')\, g(\tau')(-d\tau') \\ &= \int_{-\infty}^{\infty} g(\tau) f(x-\tau)\, d\tau = g(x) * f(x) \end{aligned} \tag{53}$$

G. *Some of the basic theorems*

1. *Initial comments*

Fourier analysis has some key theorems that provide insight into finding and understanding Fourier transforms. We describe some of these theorems below. There are more. The names and derivations of these theorems may vary somewhat from author to author. For data denoising, the most important of these is the convolution theorem. The other theorems provide the reader with useful context for Fourier theory and show how to manipulate the Fourier integral. Problems in Fourier theory that may be difficult to solve by themselves sometimes become trivial when one of these theorems is applied to them.

2. Addition, Sum, or Linearity Theorem

The addition, sum, or linearity theorem states that if $g(x)$ and $h(x)$ are functions in direct space, $G(s)$ and $H(s)$ are their Fourier transforms, and a and b are constants: $\mathcal{F}\{ag(x) + bh(x)\} = aG(s) + bH(s)$. In other words, $\mathcal{F}$, which represents the Fourier transformation, is a linear operator.

The proof of the addition or linearity theorem is quite straightforward. Consider $f(x) = ag(x) + bh(x)$, which we insert into the Fourier integral (Equation 6) to obtain:

$$
\begin{aligned}
F(s) &= \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx}dx = \int_{-\infty}^{\infty} (ag(x) + bh(x))e^{-i2\pi sx}dx \\
&= \int_{-\infty}^{\infty} ag(x)e^{-i2\pi sx}dx + \int_{-\infty}^{\infty} bh(x)\, e^{-i2\pi sx}dx \\
&= a\int_{-\infty}^{\infty} g(x)e^{-i2\pi sx}dx + b\int_{-\infty}^{\infty} h(x)\, e^{-i2\pi sx}dx \\
&= aG(s) + bH(s)
\end{aligned}
\tag{54}
$$

3. Shift Theorem

The shift theorem tells us that $\mathcal{F}\{f(x \pm a)\} = e^{\pm i2\pi sa}F(s)$. That is, shifting a function by $\pm a$ along the x-axis results in the same Fourier transform, but multiplied by $e^{\pm i2\pi sa}$.

Consider a function, $f(x)$, with a Fourier transform, $F(s)$. We now make a new function by shifting $f(x)$ to the right by an amount a, where a is a finite, positive constant, to produce: $f(x-a)$. The shift theorem reveals the relationship between the Fourier transforms of $f(x)$ and $f(x-a)$. The trick to this theorem is to define a new variable $x' = x - a$, which implies that $dx = dx'$. We begin with $f(x-a)$ in Equation 6:

$$\int_{-\infty}^{\infty} f(x-a)e^{-i2\pi sx}dx \tag{55}$$

and then substitute in $x' + a$ for x, which gives us:

$$\int_{-\infty}^{\infty} f(x')e^{-i2\pi s(x'+a)}dx' = \int_{-\infty}^{\infty} f(x')e^{-i2\pi sx'}e^{-i2\pi sa}dx' \tag{56}$$

The limits of integration remain the same because a is a finite constant. Recognizing that the $e^{-i2\pi sa}$ term is a constant in the second integral in Equation 56, and also that x' is a dummy variable, we remove $e^{-i2\pi sa}$ from the integral and replace x' with x, writing:

$$e^{-i2\pi sa}\int_{-\infty}^{\infty} f(x)e^{-i2\pi sx}dx = e^{-i2\pi sa}F(s) \tag{57}$$

Similarly, for $f(x+a)$ with $a > 0$, which shifts the function to the left, we substitute with $x' = x + a$ and $\mathrm{d}x' = dx$, which again keeps the limits of integration the same, obtaining:

$$\begin{aligned}\int_{-\infty}^{\infty} f(x+a)e^{-i2\pi sx}dx &= \int_{-\infty}^{\infty} f(x')e^{-i2\pi s(x'-a)}\,dx' \\ &= e^{i2\pi sa}\int_{-\infty}^{\infty} f(x')e^{-i2\pi sx'}\,dx' = e^{i2\pi sa}F(s)\end{aligned} \tag{58}$$

Thus, the Fourier transform of the shifted function $f(x \pm a)$ is the same as the Fourier transform of the unshifted function, but multiplied by $e^{\pm i2\pi sa}$, i.e., $\mathcal{F}\{f(x \pm a)\} = e^{\pm i2\pi sa}F(s)$.

4. Convolution Theorem

The convolution theorem tells us that the convolution of two functions in one domain is equivalent to multiplication of their Fourier transforms in the other domain, i.e., $\mathcal{F}\{f(x) * g(x)\} = F(s)G(s)$. This theorem often allows us to replace a computationally expensive convolution in direct space with a multiplication in reciprocal space.

We begin our proof of the convolution theorem by rewriting Equation 51, which defines the convolution of two functions, $f(x)$ and $g(x)$.

$$f(x) * g(x) = \int_{-\infty}^{\infty} f(\tau)\, g(x-\tau) d\tau \tag{59}$$

We now consider the Fourier transform of $f(x) * g(x)$, as follows:

$$\mathcal{F}\{f(x) * g(x)\} = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} f(\tau)\, g(x-\tau)\, d\tau \right] e^{-i2\pi sx} dx \tag{60}$$

Reversing the order of integration gives us:

$$\mathcal{F}\{f(x) * g(x)\} = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} g(x-\tau)\, e^{-i2\pi sx} dx \right] f(\tau)\, d\tau \tag{61}$$

We use the shift theorem (Equations 56 and 57) to solve the inner integral in Equation 61, which gives us:

$$\mathcal{F}\{f(x) * g(x)\} = \int_{-\infty}^{\infty} \left[G(s)e^{-i2\pi s\tau}\right] f(\tau)\, d\tau \tag{62}$$

Noting that $G(s)$ is a constant in this integral and rearranging the terms in this equation slightly completes the proof, as follows:

$$\mathcal{F}\{f(x) * g(x)\} = G(s) \int_{-\infty}^{\infty} f(\tau)\, e^{-i2\pi s\tau}\, d\tau = F(s)G(s) \tag{63}$$

Again, convolution itself, which involves reversing a function and moving it to every possible position relative to the other unshifted and unreversed function and multiplying the functions together and finding an area at each shift, can be a computationally expensive process. The convolution integral allows us to do a multiplication in reciprocal space instead. Furthermore, this possibility of multiplying in reciprocal space allows us to directly work with and manipulate the frequency content of a function.

As already suggested, the opposite of Equation 63 can also be shown. That is: $\mathcal{F}\{f(x)g(x)\} = F(s) * G(s)$. This derivation is left for the interested reader. That is, multiplication in one domain (either domain) is the same as convolution in the other.

5. Differentiation (Derivative) Theorem

If we know a function, $f(x)$, and its Fourier transform, $F(s)$, this theorem tells us that $\mathcal{F}\left(\frac{df(x)}{dx}\right) = i2\pi sF(s)$. In other words, differentiation in one domain is the same as multiplication in the other domain.

We approach this theorem by considering $f(x)$ to be the inverse Fourier transform of $F(s)$, as follows:

$$f(x) = \mathcal{F}^{-1}\{F(s)\} = \int_{-\infty}^{\infty} F(s)\, e^{i2\pi sx}\, ds \tag{64}$$

We first take the derivative of Equation 64:

$$\frac{df(x)}{dx} = \frac{d\,\mathcal{F}^{-1}\{F(s)\}}{dx} = \frac{d}{dx}\int_{-\infty}^{\infty} F(s)\, e^{i2\pi sx}\, ds \tag{65}$$

and then switch the order of differentiation and integration:

$$\frac{df(x)}{dx} = \frac{d}{dx}\int_{-\infty}^{\infty} F(s)\, e^{i2\pi sx}\ ds = \int_{-\infty}^{\infty} F(s)\left(\frac{d}{dx} e^{i2\pi sx}\right) ds \tag{66}$$

$$= \int_{-\infty}^{\infty} i2\pi s\, F(s)\, e^{i2\pi sx} ds$$

Equations 65 and 66 are equivalent to writing $\mathcal{F}\left(\frac{df(x)}{dx}\right) = i2\pi sF(s)$, so our proof is complete.

This process can be repeated, i.e., if we differentiate $f(x)$ n times to produce $\frac{d^n f(x)}{dx^n}$, its Fourier transform is: $\mathcal{F}\left(\frac{d^n f(x)}{dx^n}\right) = (i2\pi s)^n F(s)$.

These results imply that $\mathcal{F}\left(\frac{d^n f(x)}{dx^n}\right)|_{s=0} = (i2\pi s)^n F(s)\,|_{s=0} = 0$. That is, if we know $f(x)$ and $F(s)$, we know that the Fourier transforms of $f'(x)$ and also of higher derivatives of $f(x)$ are zero at $s = 0$.

6. An Aside: Fractional Derivatives: Some Advanced Mathematics Based on the Derivative Theorem

Of course, along with integrals, derivatives are a central topic in calculus. Given a function $f(x)$, we can think about its first derivative, $\frac{df(x)}{dx}$, which gives the slope of the function, the second derivative, $\frac{d^2 f(x)}{dx^2}$, which gives its curvature, all the way up to an n[th] derivative: $\frac{d^n f(x)}{dx^n}$. We can also represent differentiation via an operator, e.g., D, such that $\frac{df(x)}{dx} = D^1 f$, $\frac{d^2 f(x)}{dx^2} = D^2 f$, $\frac{d^n f(x)}{dx^n} = D^n f$, etc., and $D^0 f = f$, where D^0 means that no differentiation has taken place. It is an identity operator.

For a long time, mathematicians have wondered what a fractional derivative might look like. That is, could $D^{0.5} f$ or $D^{0.377} f$ have any reasonable meaning? The derivative theorem in Fourier analysis provides a way to define fractional derivatives. We just learned that $\mathcal{F}\left(\frac{d^n f(x)}{dx^n}\right) = (i2\pi s)^n F(s)$, which is the same as writing $\frac{d^n f(x)}{dx^n} = \mathcal{F}^{-1}((i2\pi s)^n F(s))$. If we relax the requirement that n be an integer, rather we work with a real number, say a, where $a > 0$. Then we see that $\frac{d^a f(x)}{dx^a} = D^a f = \mathcal{F}^{-1}((i2\pi s)^a F(s))$. That is, while it may not be clear how to find $D^a f$, $\mathcal{F}^{-1}((i2\pi s)^a F(s))$ is something that can be calculated, which, again, gives meaning to the idea of a fractional derivative.

7. Similarity Theorem

Assume that we know a function, $f(x)$, and its Fourier transform, $F(s)$. The similarity theorem tells us about the Fourier transform of $f(ax)$, where a is a real constant. This theorem reveals some of the reciprocal nature of the Fourier transform. We will consider separately the cases of $a > 0$ and $a < 0$ and then combine them in our final result.

Consider $a > 0$ and $\mathcal{F}\big(f(ax)\big)$. First:

$$\mathcal{F}\big(f(ax)\big) = \int_{-\infty}^{\infty} f(ax)\, e^{-i2\pi sx}\, dx \tag{67}$$

We now define a new variable, x', as $x' = ax$. Thus, $dx' = adx$, where the limits of integration do not flip because $a > 0$. Substituting and performing the appropriate mathematical operations gives us:

$$\int_{-\infty}^{\infty} f(ax)\, e^{-i2\pi sx}\, dx = \int_{-\infty}^{\infty} f(x')\, e^{-i2\pi s\left(\frac{x'}{a}\right)}\, \frac{dx'}{a} = \int_{-\infty}^{\infty} f(x')\, e^{-i2\pi\left(\frac{s}{a}\right)x'}\, \frac{dx'}{a} \tag{68}$$

$$= \frac{1}{a}\int_{-\infty}^{\infty} f(x')\, e^{-i2\pi\left(\frac{s}{a}\right)x'} dx' = \frac{1}{a} F\left(\frac{s}{a}\right)$$

Now consider $a < 0$ and $\mathcal{F}\big(f(ax)\big)$. Again:

$$\mathcal{F}\big(f(ax)\big) = \int_{-\infty}^{\infty} f(ax)\, e^{-i2\pi sx}\, dx \tag{69}$$

and we again define a new variable, x', as $x' = ax$. Thus, $dx' = adx$, but this time the limits of integration do flip because $a < 0$. Substituting and performing the appropriate mathematical operations gives us:

$$\int_{-\infty}^{\infty} f(ax)\, e^{-i2\pi sx}\, dx = \int_{\infty}^{-\infty} f(x')\, e^{-i2\pi s\left(\frac{x'}{a}\right)} \frac{dx'}{a} = \frac{1}{a}\int_{\infty}^{-\infty} f(x')\, e^{-i2\pi\left(\frac{s}{a}\right)x'} dx' \tag{70}$$

$$= -\frac{1}{a}\int_{-\infty}^{\infty} f(x')\, e^{-i2\pi\left(\frac{s}{a}\right)x'} dx' = -\frac{1}{a} F\left(\frac{s}{a}\right)$$

However, since $a < 0$, $-\frac{1}{a} > 0$, which allows us to rewrite the results from both cases as:

$$\mathcal{F}\big(f(ax)\big) = \frac{1}{|a|} F\left(\frac{s}{a}\right) \tag{71}$$

which completes our proof. Thus, any scaling we do in direct space, i.e., via $'a'$ in ax in $f(ax)$, is the opposite of what happens in reciprocal space, i.e., via $'\frac{1}{a}'$ in $\frac{s}{a}$ in $F\left(\frac{s}{a}\right)$. Note also the scaling/normalization that takes place via the $\frac{1}{|a|}$ factor.

8. *Derivative of a Convolution Integral*

This theorem says that that for two functions, $f(x)$ and $g(x)$, $\frac{d}{dx}\big(f(x) * g(x)\big) = f'(x) * g(x) = f(x) * g'(x)$. That is, the derivative of the convolution of two functions is the convolution of one of the functions with the derivative of the other.

We begin this proof by noting that if $f(x)$ and $g(x)$ have Fourier transforms of $F(s)$ and $G(s)$, the convolution theorem tells us that $\mathcal{F}\big(f(x) * g(x)\big) = F(s)G(s)$. We next use the derivative theorem, which tells us that $\mathcal{F}\left(\frac{d}{dx}\left(f(x) * g(x)\right)\right) = i2\pi s(F(s)G(s))$. Basic algebra and the convolution theorem then allow us to conclude that:

$$\mathcal{F}\left(\frac{d}{dx}\left(f(x) * g(x)\right)\right) = i2\pi s(F(s)G(s)) = \left(i2\pi sF(s)\right)G(s)$$
$$= \mathcal{F}\left(f'(x) * g(x)\right) = F(s)\left(i2\pi sG(s)\right) = \mathcal{F}\left(f(x) * g'(x)\right) \tag{72}$$

Thus, $\frac{d}{dx}\left(f(x) * g(x)\right) = f'(x) * g(x) = f(x) * g'(x)$.

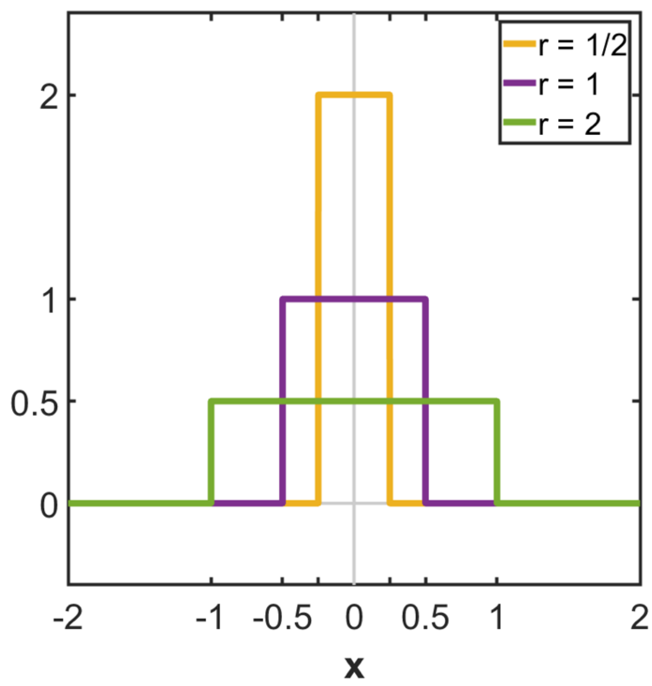

Figure 10. The boxcar function, $\frac{1}{r}\Pi\left(\frac{x}{r}\right)$, *for* $r = \frac{1}{2}, 1,$ *and* 2.

H. *The impulse (delta) function*

The impulse function, or delta function, is defined as

$$\delta(x) = 0 \; for \; x \neq 0 \tag{73}$$

and

$$\int_{-\infty}^{\infty} \delta(x)\, dx = 1 \tag{74}$$

Thus, the impulse or delta function captures the idea of an infinitely narrow function that has an area of unity. Accordingly, the delta function is a function that exists in a limit, where there are infinitely many approximating sequences of functions that can be defined to meet the conditions outlined in Equations 73 and 74. Technically speaking, the delta function is referred to as a generalized function.

For example, we will now create a delta function based on a boxcar function. To do this, let's first consider $\Pi\left(\frac{x}{r}\right)$, where r is a parameter that we control. From our definition of the boxcar function, we recognize that $\Pi\left(\frac{x}{r}\right)$ will be unity between $\frac{x}{r} = -\frac{1}{2}$ and $\frac{x}{r} = \frac{1}{2}$, i.e., between $x = -\frac{r}{2}$ and $x = \frac{r}{2}$. That is, the width of the boxcar function $\Pi\left(\frac{x}{r}\right)$ is r. It is zero everywhere else.

We now imagine allowing r in $\Pi\left(\frac{x}{r}\right)$ to become very small. However, this alone does not make $\Pi\left(\frac{x}{r}\right)$ into a delta function. Rather, if $r \to 0$, we obtain a null function:

$$\delta^0(x) = \lim_{r \to 0} \Pi\left(\frac{x}{r}\right) \tag{75}$$

We can confirm that we have a null function by integrating Equation 75, which gives:

$$\int_{-\infty}^{\infty} \lim_{r\to 0} \Pi\left(\frac{x}{r}\right) dx = \lim_{r\to 0} \int_{-\frac{r}{2}}^{\frac{r}{2}} 1\, dx = \lim_{r\to 0} r = 0 \tag{76}$$

We know that the width, and area, of the rectangle defined by $\Pi\left(\frac{x}{r}\right)$ is r. Accordingly, we could keep the area of a function based on $\Pi\left(\frac{x}{r}\right)$ constant, and unity, if we multiplied it by $\frac{1}{r}$. Accordingly, a definition of the delta function is:

$$\delta(x) = \lim_{r\to 0} \frac{1}{r} \Pi\left(\frac{x}{r}\right) \tag{77}$$

Where, the height of this function, $\frac{1}{r}$, does indeed go to infinity and its width, r, goes to zero. Figure 10 shows a few examples of $\frac{1}{r}\Pi\left(\frac{x}{r}\right)$ for different values of r. Delta functions can also be defined from triangle, Gaussian, and Lorentzian functions, where these functions will be discussed/mentioned below. Sometimes it is advantageous to be able to differentiate the delta function. Defining the delta function in terms of a triangle function gives us one derivative we can work with, whereas defining it in terms of a Gaussian gives us infinitely many derivatives.

As defined in Equations 73 – 74, the delta function is an even function, i.e., $\delta(x) = \delta(-x)$.

The delta function behaves in an interesting fashion in integrals with other functions. It picks out the value of the function that is in an integral. Let's first consider:

$$\int_{-\infty}^{\infty} \delta(x) f(x)\, dx \tag{78}$$

We recall that the delta function, $\delta(x)$, is zero everywhere except at zero, so the only place where $\delta(x)f(x)$ is not zero is at $x = 0$. Thus, for a function that is continuous at the origin:

$$\int_{-\infty}^{\infty} \delta(x) f(x)\, dx = \int_{-\infty}^{\infty} \delta(x) f(0)\, dx \tag{79}$$

That is, $f(x)$ approaches the constant value of $f(0)$ as $x \to 0$, so it can be taken out of the integral, and the remaining integral, which is just the integral of $\delta(x)$, is unity, so we can write:

$$\int_{-\infty}^{\infty} \delta(x) f(x)\, dx = \int_{-\infty}^{\infty} \delta(x) f(0)\, dx = f(0) \int_{-\infty}^{\infty} \delta(x)\, dx = f(0) \tag{80}$$

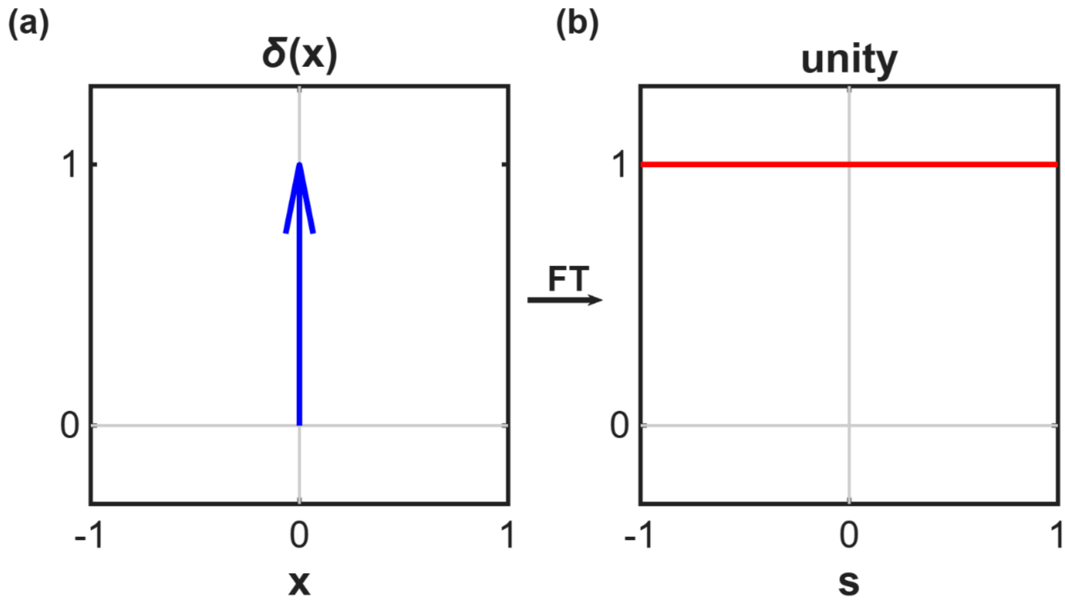

Figure 11. (a) Representation of the delta function, $\delta(x)$, and (b) its Fourier transform, which is unity. Note that in (a), the y-axis scale refers to the area of the delta function, not its height!

In a document like this one, one might inquire about the Fourier transform of the delta function. It is easily calculated as follows:

$$\int_{-\infty}^{\infty} \delta(x) e^{-i2\pi sx} dx = e^{0} \int_{-\infty}^{\infty} \delta(x) dx = 1 \tag{81}$$

In other words, $\mathcal{F}\big(\delta(x)\big) = 1$ (see Figure 11). Similarly, we can find the Fourier transform of a shifted delta function, $\delta(x-a)$, as follows:

$$F(s) = \int_{-\infty}^{\infty} \delta(x-a) e^{-i2\pi sx} dx = e^{-i2\pi sa} \int_{-\infty}^{\infty} \delta(x) dx = e^{-i2\pi sa} \tag{82}$$

Again, in an integral, the delta function picks out the value of the function at the point where the delta function is not zero.

The Fourier transform pair of $\delta(x)$ and 1 has an interesting graphical interpretation. The implication is that an infinitely narrow and sharp function, the delta function, is made up of equal amounts of all possible frequencies.

An important property of the delta function is its behavior in convolution. That is, what is $\delta(x) * f(x)$? To perform this calculation, we return to the definition of convolution:

$$\delta(x) * f(x) = \int_{-\infty}^{\infty} \delta(\tau) f(x-\tau)\, d\tau = f(x) \int_{-\infty}^{\infty} \delta(\tau)\, d\tau = f(x) \tag{83}$$

Thus, the convolution of any function with the delta function is the function itself. The delta function is an identity element for convolution, behaving in convolution like unity does in multiplication.

As an extension to the ideas in the last paragraph, we consider the convolution of a function with a shifted delta function, $\delta(x-a)$:

$$\begin{aligned} &\delta(x-a) * f(x) \\ &\quad = \int_{-\infty}^{\infty} \delta(\tau - a) f(x-\tau)\, d\tau \\ &\quad = f(x-a) \int_{-\infty}^{\infty} \delta(\tau - a)\, d\tau = f(x-a) \end{aligned} \tag{84}$$

Thus, the convolution of a function with a shifted delta function shifts the function by the same amount that the delta function was shifted by.

Another property of the delta function that should be remembered is that:

$$\delta(x) = \frac{1}{|a|}\delta(ax) \tag{85}$$

We can demonstrate this property from the boxcar definition of the delta function that we used above:

$$\int_{-\infty}^{\infty} \delta(x)dx = \int_{-\infty}^{\infty} \lim_{r\to 0} \frac{1}{r}\Pi\left(\frac{x}{r}\right) dx \tag{86}$$

Thus, for $\delta(ax)$ we write:

$$\int_{-\infty}^{\infty} \delta(ax)dx = \int_{-\infty}^{\infty} \lim_{r\to 0} \frac{1}{r}\Pi\left(\frac{ax}{r}\right) dx \tag{87}$$

Let's consider first the case of $a > 0$ and substitute $x' = ax$ into this equation, which means that $dx' = adx$ and the limits of integration stay the same because $a > 0$:

$$\int_{-\infty}^{\infty} \delta(ax)dx = \int_{-\infty}^{\infty} \lim_{r\to 0} \frac{1}{r}\Pi\left(\frac{x'}{r}\right)\frac{dx'}{a} = \int_{-\infty}^{\infty} \left(\frac{1}{a}\right)\lim_{r\to 0} \frac{1}{r}\Pi\left(\frac{x'}{r}\right)dx' \tag{88}$$

$$= \int_{-\infty}^{\infty} \left(\frac{1}{a}\right)\delta(x)dx$$

For $a < 0$, we again substitute $x' = ax$ into Equation 87, which means that $dx' = adx$, and the limits of the integral are reversed:

$$\int_{-\infty}^{\infty} \delta(ax)dx = \int_{\infty}^{-\infty} \lim_{r\to 0} \frac{1}{r}\Pi\left(\frac{x'}{r}\right)\frac{dx'}{a} = \left(-\frac{1}{a}\right)\int_{-\infty}^{\infty} \lim_{r\to 0} \frac{1}{r}\Pi\left(\frac{x'}{r}\right)dx' \tag{89}$$

$$= \left(-\frac{1}{a}\right)\int_{-\infty}^{\infty} \delta(x)dx$$

The results in the integrals in Equations 88 and 89 thus imply that $\delta(ax) = \frac{1}{|a|}\delta(x)$.

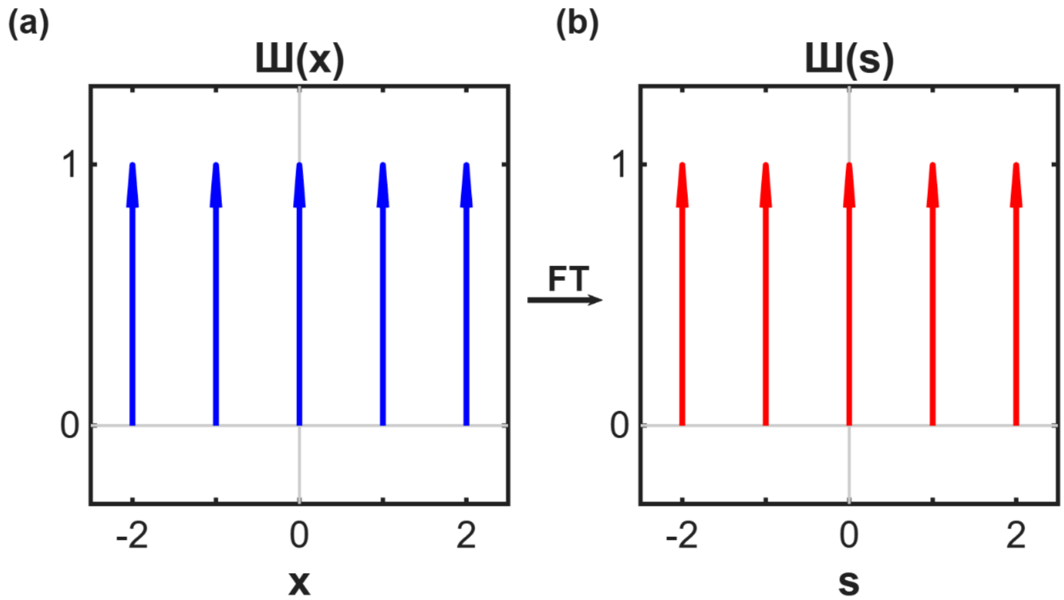

Figure 12. The central part of the shah function in direct space, Ш(x)*, and (b) the central part of its Fourier transform* Ш(s)*.*

I. *The shah (comb) function*

The shah function, Ш(x), which is shown in Figure 12, is an infinite set of delta functions spaced at unit intervals across the x-axis, as follows:

$$\text{Ш}(x) = \sum_{n=-\infty}^{\infty} \delta(x - n) \tag{90}$$

where n is an integer. The symbol for this function, Ш, has Cyrillic roots, which relates it to the Hebrew letter ש (sin/shin), which in turn is derived from a Phoenician letter of similar shape. The point here is that the three columns or peaks or spikes (however you wish to view it) in the letter Ш are meant to resemble a series of delta functions, where we often depict a single delta function graphically as a spike.

The shah function is a sampling function. When it is multiplied by a function that is well-behaved at integer values, it picks out the values of the function at the integer values. Thus, the shah function turns a continuous function, $f(x)$, into a discrete function, $Ш(x)f(x)$, as follows:

$$
\begin{aligned}
Ш(x)f(x) &= \left(\sum_{n=-\infty}^{\infty} \delta(x-n)\right) f(x) \\
&= \sum_{n=-\infty}^{\infty} f(x)\delta(x-n) = \sum_{n=-\infty}^{\infty} f(n)\delta(x-n)
\end{aligned}
\tag{91}
$$

Obviously, it would be nice to be able to change the spacing between the delta function in the shah function. We can do this through $Ш(ax)$. From the theory developed in this document we can write:

$$
Ш(ax) = \sum_{n=-\infty}^{\infty} \delta(ax-n) = \sum_{n=-\infty}^{\infty} \delta\left(a\left(x-\frac{n}{a}\right)\right) = \frac{1}{|a|}\sum_{n=-\infty}^{\infty} \delta\left(x-\frac{n}{a}\right)
\tag{92}
$$

Thus, by changing a in $Ш(ax)$, we change the spacing between the delta functions in our $Ш(ax)$ function compared to $Ш(x)$, where the spacing becomes $\frac{1}{|a|}$.

In the previous section of this document, we learned that: $\delta(x-a) * f(x) = f(x-a)$. We can now ask what happens when we convolve the shah function with another function.

$$f(x) * Ш(ax) = f(x) * \sum_{n=-\infty}^{\infty} \frac{1}{|a|} \delta\left(x - \frac{n}{a}\right) = \sum_{n=-\infty}^{\infty} f(x) * \frac{1}{|a|} \delta\left(x - \frac{n}{a}\right) = \frac{1}{|a|} \sum_{n=-\infty}^{\infty} f\left(x - \frac{n}{a}\right) \tag{93}$$

That is, the convolution of the shah function with a function, $f(x)$, creates an infinite number of shifted copies of $f(x)$ that are scaled by $\frac{1}{|a|}$. The shah function is a replicating function. Note that these copies of a function may overlap.

Here's an example of $Ш(x)$ as a replicating a function. We could define a slightly asymmetric boxcar function, $\Pi_c(x)$, as:

$$\Pi_c(x) = \begin{cases} 0, for\ x \leq -\frac{1}{2} \\ 1, for\ -\frac{1}{2} < x \leq \frac{1}{2} \\ 0, for\ x > \frac{1}{2} \end{cases} \tag{94}$$

where $Ш(x) * \Pi_c(x) = 1$.

Of course,

$$\int_{n-1/2}^{n+1/2} Ш(x)\, dx = 1, for\ all\ integers\ n \tag{95}$$

More thoroughly, we could write:

$$\int_{n-a}^{n+a} Ш(x)\, dx = 1, for\ all\ integers\ n\ and\ 0 < a < 1 \tag{96}$$

The Fourier transform of a shah function is another shah function. This important result will be discussed in the next section on Fourier transform pairs.

J. *Some common Fourier transform pairs*

1. Initial Comments

The following transform pairs are important in Fourier theory. We will denote a Fourier transform pair in this section, i.e., a function and its Fourier transform, with a double-headed arrow.

Before presenting a list of transform pairs, we discuss an important result regarding the transform pairs of even functions.

2. The transform pairs of even functions.

As noted above, the Fourier transforms of an even function is an even function. In addition, because of Euler's relationship and the properties of even and odd functions, for an even function, $E(x)$:

$$\int_{-\infty}^{\infty} E(x)e^{-i2\pi sx}dx = \int_{-\infty}^{\infty} E(x)\, e^{i2\pi sx}dx = \int_{-\infty}^{\infty} E(x)\, cos(2\pi sx)\, dx \tag{97}$$

In other words, we get the same answer with either $e^{-i2\pi sx}$ or $e^{i2\pi sx}$.

We can write a Fourier transform pair of an even function in direct space, $E_{dir}(x)$, and its Fourier transform in reciprocal space, $E_{rec}(s)$, as $E_{dir}(x) \leftrightarrow E_{rec}(s)$, or using the definition of the forward Fourier transform:

$$\int_{-\infty}^{\infty} E_{dir}(x)e^{-i2\pi sx}dx = E_{rec}(s) \tag{98}$$

Alternatively, we can write the inverse transform connecting these even functions as:

$$E_{dir}(x) = \int_{-\infty}^{\infty} E_{rec}(s)e^{i2\pi sx}ds \tag{99}$$

But it doesn't matter what we call x and s in Equation 99, so we can switch x and s to obtain:

$$E_{dir}(s) = \int_{-\infty}^{\infty} E_{rec}(x)e^{i2\pi sx}dx \tag{100}$$

Equation 97 then allows us to write:

$$E_{dir}(s) = \int_{-\infty}^{\infty} E_{rec}(x) e^{-i2\pi sx} dx \tag{101}$$

Thus, we see that:

$$\text{If } E_{dir}(x) \leftrightarrow E_{rec}(s) \text{ then } E_{rec}(x) \leftrightarrow E_{dir}(s). \tag{102}$$

For example, because $\Pi(x)$ is an even function and $\Pi(x) \leftrightarrow sinc(s)$, then $sinc(x) \leftrightarrow \Pi(s)$.

We bring up this fact because a number of the Fourier transform pairs discussed below involve even functions. Thus, by Equation 102 we have two transform pairs for each Fourier transform pair that involves an even function.

3. The boxcar-sinc pair

This important Fourier transform pair $\Pi(x) \leftrightarrow sinc(s)$ was discussed above. It is shown in Figure 5. From Equation 102, it is also true that $sinc(x) \leftrightarrow \Pi(s)$. We will not repeat this relationship for the transform pairs of the other even functions below. Note that the Fourier transform of $sinc(x)$, which is $\Pi(s)$, is non-zero only over a limited set of frequencies. Functions with this property are said to be 'band-limited'.

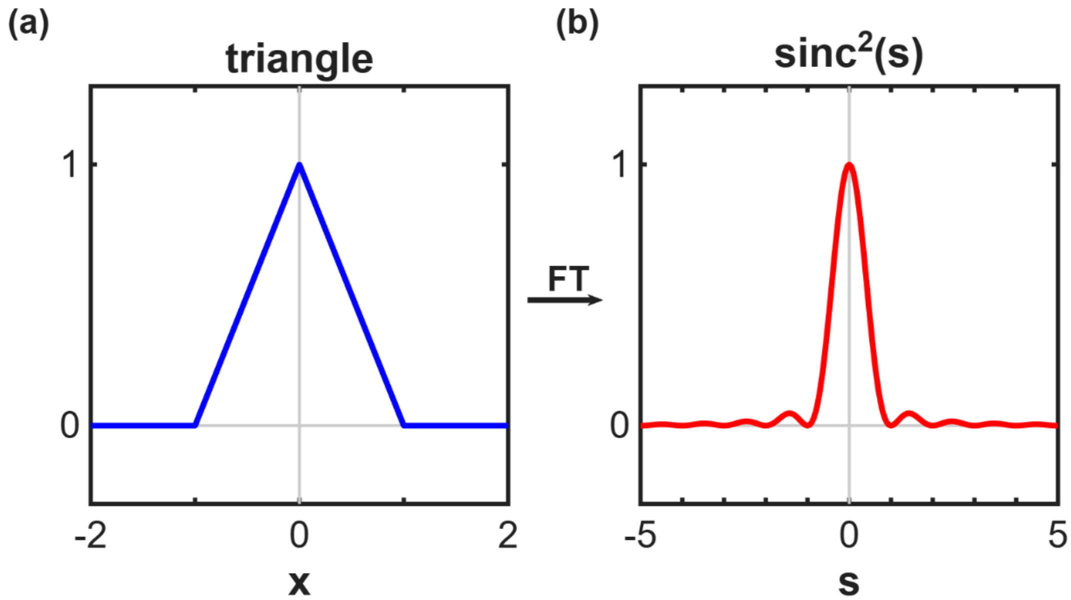

Figure 13. (a) The triangle function, $\Lambda(x)$, and (b) Its Fourier transform $sinc^2(s)$.

4. The triangle function-sinc² pair

The boxcar function, $\Pi(x)$, was defined in Equation 11 above, where its Fourier transform is $sinc(s)$. Convolving a boxcar function with itself, $\Pi(x) * \Pi(x)$, yields the triangle function, $\Lambda(x)$, which is defined as:

$$\Lambda(x) = \begin{cases} 1 - |x|, & |x| \leq 1 \\ 0, & |x| > 1 \end{cases} \tag{103}$$

Notice that, as is typical in convolution, $\Lambda(x)$ is broader and smoother than $\Pi(x)$. As an aside, if we continue to convolve $\Pi(x)$ with itself, we will get a broader and smoother function, which, according to the central limit theorem, will approach a Gaussian. Even $\Pi(x) * \Pi(x) * \Pi(x)$, and especially $\Pi(x) * \Pi(x) * \Pi(x) * \Pi(x)$, resemble a Gaussian to a surprising degree. From the convolution theorem, we know that convolution in one domain is the same as multiplication in the other. Accordingly, $\mathcal{F}\big(\Lambda(x)\big) = \mathcal{F}\big(\Pi(x) * \Pi(x)\big) = sinc(s) \cdot sinc(s) = sinc^2(s)$. This transform pair ($\Lambda(x) \leftrightarrow sinc^2(s)$) is shown in Figure 13.

5. *Delta function-unity pair, and also the pair for the shifted delta function*

As noted above, and shown in Figure 11, the Fourier transform of the delta function, $\delta(x)$, is unity, i.e., $\delta(x) \leftrightarrow 1$, and for the shifted delta function we have $\delta(x-a) \leftrightarrow e^{-i2\pi sa}$.

As just noted, $\delta(x) \leftrightarrow 1$ implies $1 \leftrightarrow \delta(s)$. How might we rationalize this? What follows is not a mathematically rigorous proof, but rather some plausibility arguments. First, for $1 \leftrightarrow \delta(s)$, we can write:

$$F(s) = \int_{-\infty}^{\infty} 1 \cdot e^{-i2\pi sx} dx \tag{104}$$

We then note that, under these symmetric limits (from $-\infty$ to ∞), all the sine components of $e^{-i2\pi sx}$ are zero. Thus, Equation 104 becomes:

$$F(s) = \int_{-\infty}^{\infty} 1 \cdot \cos(2\pi sx) dx \tag{105}$$

We now consider two scenarios for Equation 105. In the first case, $s = 0$, which gives:

$$F(0) = \int_{-\infty}^{\infty} 1dx \tag{106}$$

which implies that $F(0)$ is infinity. In the second case, we consider $s \neq 0$. Technically speaking, Equation 105 doesn't converge for $s \neq 0$. Nevertheless, one could argue heuristically that the integral of $\cos(2\pi sx)$ over limits of $-\infty$ to ∞ is zero because the positive and negative parts of $\cos(2\pi sx)$ cancel. Thus, considering these two cases creates a plausibility argument for $1 \leftrightarrow \delta(s)$.

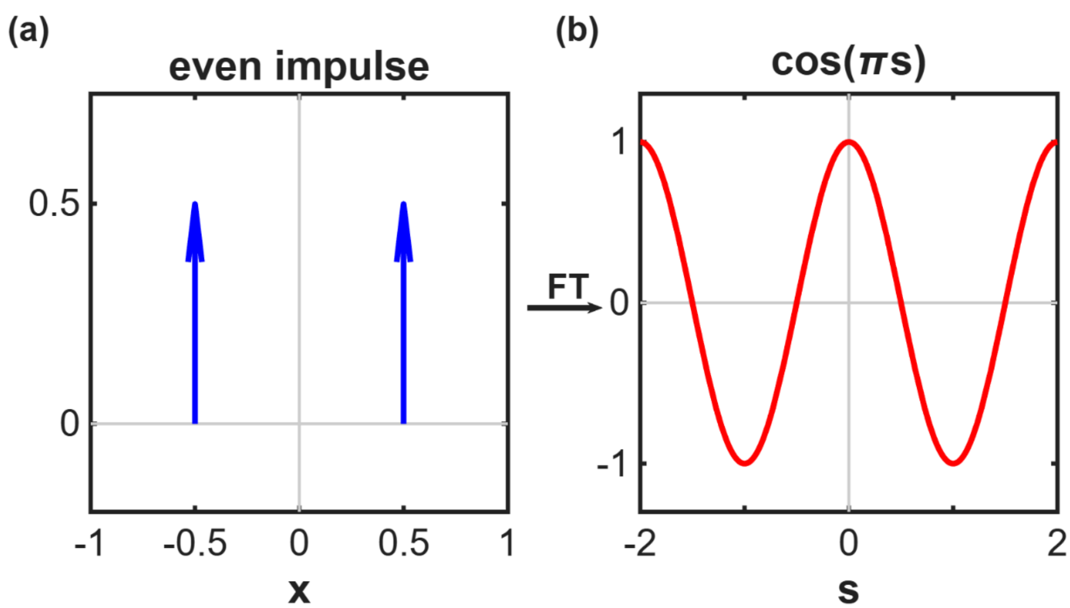

Figure 14. The (a) Even impulse pair: $II(x) = \frac{1}{2}\left(\delta\left(x+\frac{1}{2}\right) + \delta\left(x-\frac{1}{2}\right)\right)$, and (b) Cosine ($\cos(\pi s)$) Fourier transform pair.

6. *Even impulse pair-Cosine pair*

Consider the Fourier transform of the following function of two delta functions: $\frac{1}{2}\big(\delta(x+a) + \delta(x-a)\big)$, where a is a real number:

$$\frac{1}{2}\int_{-\infty}^{\infty}(\delta(x+a)+\delta(x-a))e^{-i2\pi sx}dx=\frac{1}{2}\left(e^{i2\pi sa}+e^{-i2\pi sa}\right)=cos(2\pi as) \tag{107}$$

Note that the parameter a, which gives the distance of the delta functions from the y-axis in direct space, corresponds to the frequency of the cosine in reciprocal space.

Bracewell[3] defines the $\mathrm{II}(x)$ function as $\frac{1}{2}\left(\delta\left(x+\frac{1}{2}\right)+\delta\left(x-\frac{1}{2}\right)\right)$, which, per Equation 107, has a Fourier transform of $cos(\pi s)$ (see Figure 14). This symbol (II) is obviously supposed to be reminiscent of a pair of delta functions.

In summary, $\frac{1}{2}(\delta(x+a)+\delta(x-a))\leftrightarrow cos(2\pi as)$. If we insert $a=\frac{1}{2}$ into this result we get $\mathrm{II}(x)=\frac{1}{2}\left(\delta\left(x+\frac{1}{2}\right)+\delta\left(x-\frac{1}{2}\right)\right)\leftrightarrow cos(\pi s)$, i.e., $\mathrm{II}(x)\leftrightarrow cos(\pi s)$.

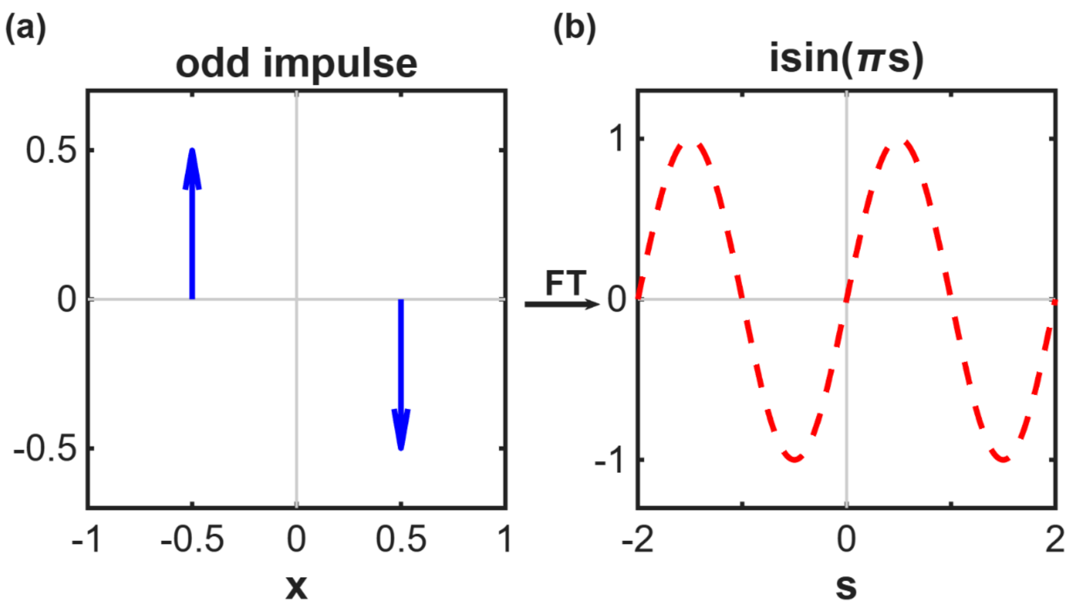

Figure 15. (a) The odd impulse pair $I_I(x)=\frac{1}{2}\left(\delta\left(x+\frac{1}{2}\right)-\delta\left(x-\frac{1}{2}\right)\right)$ and (b) its Fourier transform $isin(2\pi as)$. The dashed line reminds us that the function in (b) is imaginary.

7. Odd impulse pair-Sine pair

Consider the two delta functions, $\frac{1}{2}\left(\delta(x+a)-\delta(x-a)\right)$. Their Fourier transform can be obtained directly, as follows:

$$\frac{1}{2}\int_{-\infty}^{\infty}\left(\delta(x+a)-\delta(x-a)\right)e^{-i2\pi sx}dx=\frac{1}{2}\left(e^{i2\pi sa}-e^{-i2\pi sa}\right)=isin(2\pi as) \tag{108}$$

Again, the parameter a, which gives the distance of the delta functions from the y-axis in direct space corresponds to the frequency of the sinusoid in reciprocal space. Note also that, as expected, the Fourier transform of an odd function, $\frac{1}{2}\left(\delta(x+a)-\delta(x-a)\right)$, is an imaginary odd function.

Bracewell[3] defines the function $\mathrm{I_I}(x)$ as $\frac{1}{2}\left(\delta\left(x+\frac{1}{2}\right)-\delta\left(x-\frac{1}{2}\right)\right)$, which has a Fourier transform of $i\ sin(\pi s)$ (see Figure 15). This symbol ($\mathrm{I_I}$) is obviously supposed to be reminiscent of a pair of delta functions, where the first is positive and the second negative.

In summary, $\frac{1}{2}\left(\delta(x+a)-\delta(x-a)\right)\leftrightarrow i\ sin(2\pi as)$, and $\mathrm{I_I}(x)=\frac{1}{2}\left(\delta\left(x+\frac{1}{2}\right)-\delta\left(x-\frac{1}{2}\right)\right)\leftrightarrow i\ sin(\pi s)$, which is just the previous result with $a=\frac{1}{2}$.

8. The Fourier transform of a null function is zero (see discussion above). That is: $\delta^0(t)\leftrightarrow 0$.

Our comment about the Fourier transform pairs of even functions at the beginning of this section does not really apply here because of Lerch's theorem. That is, it is true that $\delta^0(t)$ is an even function and that $\mathcal{F}\left(\delta^0(t)\right)=0$, but the opposite $\mathcal{F}^{-1}(0)=\delta^0(t)$ is not necessarily true.

That is, $\mathcal{F}^{-1}(0)$ is certainly zero or a null function, but without more information we have no way of knowing which null function $\mathcal{F}^{-1}(0)$ corresponds to, or whether it corresponds to zero. Technically speaking, we would say that $\mathcal{F}^{-1}(0)$ is zero almost everywhere.

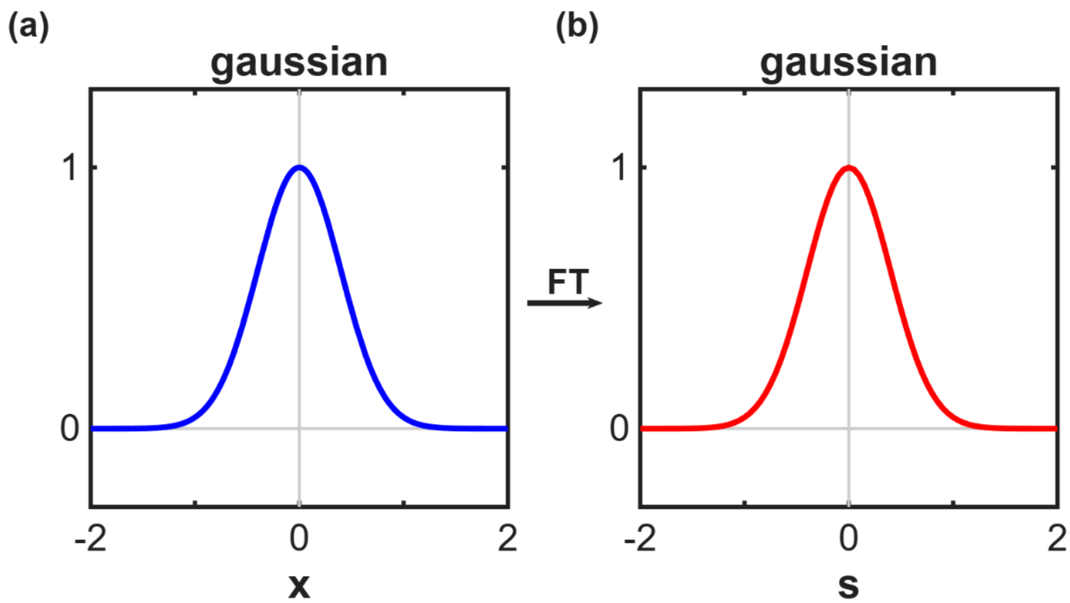

Figure 16. (a) The Gaussian $e^{-\pi x^2}$ in direct space, and (b) the Gaussian $e^{-\pi s^2}$ in reciprocal space as a Fourier transform pair.

9. *The Gaussian-Gaussian pair*

An important Fourier transform pair is $e^{-\pi x^2} \leftrightarrow e^{-\pi s^2}$, which we obtain as follows. First, we write out the Fourier transform for $e^{-\pi x^2}$, which is:

$$\int_{-\infty}^{\infty} e^{-\pi x^2} e^{-i2\pi sx} dx \tag{109}$$

Recognizing that $e^{-\pi x^2}$ is an even function, we write:

$$\int_{-\infty}^{\infty} e^{-\pi x^2} cos(2\pi sx) dx \tag{110}$$

Equation 110 can be looked up in a table of integrals and is $e^{-\pi s^2}$. Thus, $e^{-\pi x^2} \leftrightarrow e^{-\pi s^2}$.

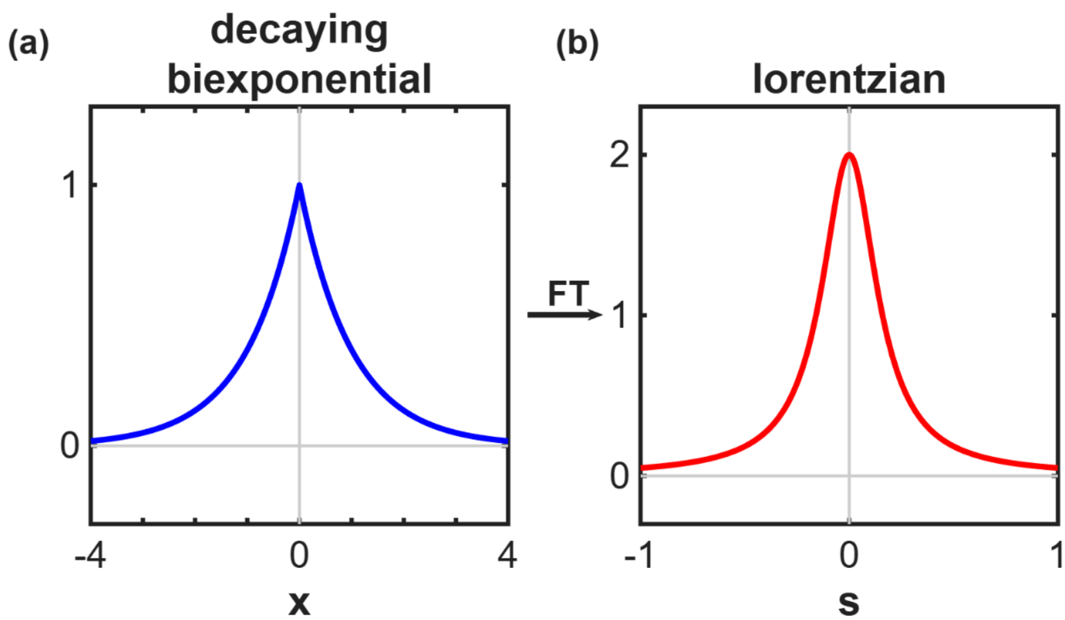

Figure 17. The (a) Decaying biexponential ($e^{-|x|}$), and (b) Lorentzian ($\frac{2}{1+4\pi^2 s^2}$) Fourier transform pair.

10. The Lorentzian-Decaying biexponential pair

We now consider the Fourier transform of $e^{-a|x|}$, where $a > 0$.

$$\int_{-\infty}^{\infty} e^{-a|x|} e^{-i2\pi sx} dx \tag{111}$$

We solve this problem by breaking this integral into two parts:

$$\int_{-\infty}^{\infty} e^{-a|x|} e^{-i2\pi sx} dx \tag{112}$$

$$= \int_{-\infty}^{0} e^{ax} e^{-i2\pi sx} dx$$

$$+ \int_{0}^{\infty} e^{-ax} e^{-i2\pi sx} dx$$

$$= \int_{-\infty}^{0} e^{(a-i2\pi s)x} dx + \int_{0}^{\infty} e^{-(a+i2\pi s)x} dx = \frac{1}{a - i2\pi s} e^{(a-i2\pi s)x}\Big|_{-\infty}^{0}$$

$$+ \frac{-1}{a + i2\pi s} e^{-(a+i2\pi s)x}\Big|_{0}^{\infty} = \frac{1}{a - i2\pi s} + \frac{1}{a + i2\pi s}$$

$$= \frac{2a}{a^2 + 4\pi^2 s^2}$$

Thus, $e^{-a|x|} \leftrightarrow \frac{2a}{a^2+4\pi^2 s^2}$. Note that $\frac{2a}{a^2+4\pi^2 s^2}$ is a Lorentzian, i.e., it has the basic form $\frac{1}{1+s^2}$, so the Fourier transform of a decaying biexponential is a Lorentzian (see Figure 17).

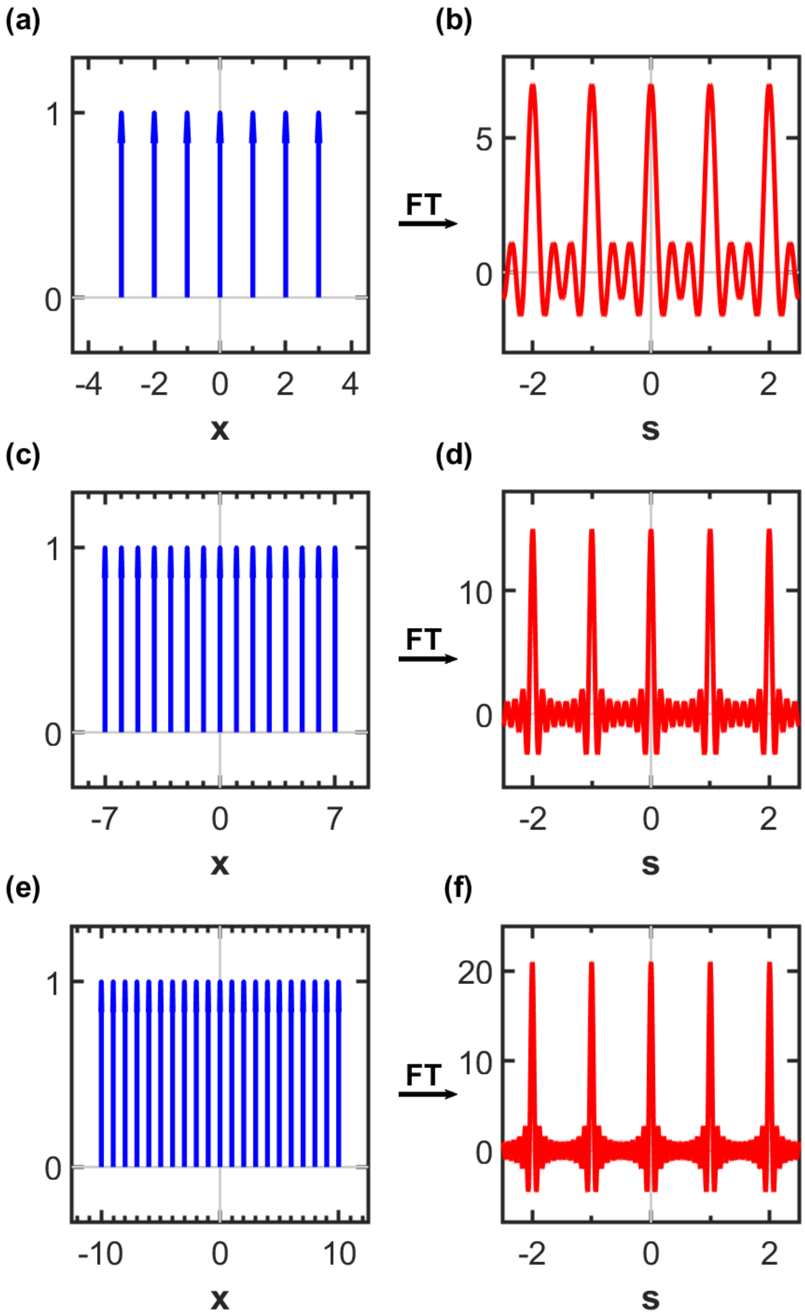

Figure 18. Justification for how the shah function can be its own Fourier transform. The results of Fourier transforming $\widetilde{\text{III}}_m(x)$*, i.e.,* $\mathcal{F}\left(\widetilde{\text{III}}_m(x)\right)$*, for (a – b)* $m = 3$*, (c – d)* $m = 7$*, (e – f) and* $m = 10$*.*

11. Shah-shah pair

It turns out that the shah function is its own Fourier transform. That is $Ш(x) \leftrightarrow Ш(s)$ (see Figure 18). We published a short tutorial article in Vacuum Technology & Coating that explains why this could be the case.[33] We took Fourier transforms of finite sums of delta function pairs around $x = 0$ (the middle of $Ш(x)$) and also the middle delta function of $Ш(x)$. That is, we considered Equation 90 over increasing, symmetric limits that were not $-\infty$ and ∞. For example, Equation 113 shows Equation 90 as a partial sum, $\widetilde{Ш}_m(x)$, extending from $-m$ to m, where m is an integer, and Figure 18 shows the results of Fourier transforming $\widetilde{Ш}_m(x)$, i.e., $\mathcal{F}\left(\widetilde{Ш}_m(x)\right)$, for $m = 3$, 7, and 10. As m increases, $\mathcal{F}\left(\widetilde{Ш}_m(x)\right)$ increasingly looks like $Ш(s)$.

$$\widetilde{Ш}_m(x) = \sum_{n=-m}^{m} \delta(x-n) \tag{113}$$

The following argument helps explain why $\mathcal{F}\left(\widetilde{Ш}_m(x)\right)$ turns into $Ш(s)$ as $m \to \infty$. First, when $m = 1$, $\widetilde{Ш}_1(x) = \delta(x) + \delta(x-1) + \delta(x+1)$ and $\mathcal{F}\left(\widetilde{Ш}_1(x)\right) = 1 + 2cos(2\pi s)$, where, in general, $\mathcal{F}\big(\delta(x-n) + \delta(x+n)\big) = 2cos(2\pi sn)$. These results mean that each cosine created by a pair of delta functions at equal distances, n, from the y-axis creates a cosine ($cos(2\pi sn)$) with a frequency that is an integer multiple of the cosine $cos(2\pi s)$, which, again, is produced by the closest two delta functions to the y-axis: $\delta(x-1)$ and $\delta(x+1)$. Because n is an integer, $cos(2\pi sn)$ has a value of unity at all integer values of s, so there is constructive interference of the $cos(2\pi sn)$ functions whenever s is an integer. As a result, we end up with infinitely high spikes where s is an integer, which leads to delta functions at these locations.

K. *The convolution of a Gaussian with a Gaussian. An example with important implications for XPS and spectroscopy in general*

1. *The convolution of a Gaussian with a Gaussian*

This subsection describes an important result that is based on the $e^{-\pi x^2} \leftrightarrow e^{-\pi s^2}$ transform pair. Let's imagine that we have two of these Gaussian-Gaussian transform pairs, which, for a and b as non-zero, positive, real constants, and based on the Similarity Theorem, are $e^{-\pi(ax)^2} \leftrightarrow \frac{1}{|a|}e^{-\pi(S/a)^2}$ and $e^{-\pi(bx)^2} \leftrightarrow \frac{1}{|b|}e^{-\pi(S/b)^2}$. What is the convolution of these two Gaussians, i.e., what is $\mathcal{F}\left(e^{-\pi(ax)^2} * e^{-\pi(bx)^2}\right)$? We invoke the convolution theorem, which tells us that $\mathcal{F}\left(e^{-\pi(ax)^2} * e^{-\pi(bx)^2}\right) = \frac{1}{|a|}e^{-\pi(S/a)^2} \cdot \frac{1}{|b|}e^{-\pi(S/b)^2} = \frac{1}{|ab|}e^{-\pi s^2\left(1/a^2+1/b^2\right)}$. We define $1/c^2 = 1/a^2 + 1/b^2$, which gives us $\frac{1}{|ab|}e^{-\pi(S/c)^2}$. Thus, after a little algebra, $\frac{|c|}{|ab|}\mathcal{F}^{-1}\left(\frac{1}{|c|}e^{-\pi(S/c)^2}\right) = \frac{|c|}{|ab|}e^{-\pi(cx)^2} = \frac{|c|}{|ab|}e^{-\pi c^2x^2}$. That is, $e^{-\pi(ax)^2} * e^{-\pi(bx)^2} = \frac{|c|}{|ab|}e^{-\pi c^2x^2}$.

2. *Conclusions we can draw from the previous section*

First, this example illustrates the important fact that the convolution of two Gaussians is another Gaussian.

Second, the convolution of two Gaussians is broader than either of the original Gaussians. We demonstrate this result as follows. From $1/c^2 = 1/a^2 + 1/b^2$ we write $c^2 = \frac{a^2b^2}{a^2+b^2}$, which allows us to also write $c^2 = \frac{a^2}{\left(\frac{a}{b}\right)^2+1}$ and $c^2 = \frac{b^2}{\left(\frac{b}{a}\right)^2+1}$. However, because $\left(\frac{a}{b}\right)^2 + 1 > 1$ and $\left(\frac{b}{a}\right)^2 + 1 > 1$, these equations imply that $c^2 < a^2$ and $c^2 < b^2$. Thus, $e^{-\pi(cx)^2}$ is broader than both $e^{-\pi(ax)^2}$ and $e^{-\pi(bx)^2}$. This conclusion is quite general. The convolution of two functions generally produces a broader function than either of the original functions. An important exception here is the convolution of a function with the delta function, which returns the original function.

Third, when a broad Gaussian is convolved with a narrow Gaussian, we basically just get the broad Gaussian back. To show this, we consider $e^{-\pi(ax)^2} * e^{-\pi(bx)^2} = \frac{|c|}{|ab|}e^{-\pi c^2x^2}$ for $a \gg b$, which means that $e^{-\pi(ax)^2}$ is much narrower than $e^{-\pi(bx)^2}$. Under these conditions, i.e., assuming a is very large, $1/_{c^2} \approx 1/_{b^2}$, which means that $e^{-\pi c^2x^2} \approx e^{-\pi b^2x^2}$. Thus, for $a \gg b$, $e^{-\pi(ax)^2} * e^{-\pi(bx)^2} \approx \frac{1}{|a|}e^{-\pi b^2x^2}$. This result has important implications for XPS. First, however, we generalize this result by stating that, in general, the convolution of a broad function with a narrow function returns something close to the broad function, perhaps multiplied by a scaling constant. Now, it is well recognized in XPS that the width of a peak can be viewed as a result of a convolution of the intrinsic peak width given by quantum mechanics, which is Lorentzian, with factors that include the width of the X-ray source and broadening from the instrument, part of which would be controlled by the pass energy. The point here is that if our intrinsic peak is a broad Lorentzian, we would basically expect to get this peak back when we collect it with a narrow monochromatic source and low pass energy. On the flip side, it will difficult not to see the effects of the X-ray source and instrument with a narrow peak.

L. *The Modulation Theorem, and the reciprocal relationship between functions and their Fourier transforms.*

1. *Modulation theorem*

From our discussion above on the 'Even impulse pair-Cosine pair', we showed that $\frac{1}{2}\big(\delta(x+a)+\delta(x-a)\big) \leftrightarrow cos(2\pi as)$. Accordingly, $\cos(2\pi at) \leftrightarrow \frac{1}{2}\big(\delta(f+a)+\delta(f-a)\big)$.

Consider a function, $f(t)$, which has a Fourier transform, $F(f)$, that is modulated (modified) with $\cos(2\pi at)$ such that $f(t)\cos(2\pi at)$. What is the Fourier transform of $f(t)\cos(2\pi at)$? To solve this problem, we invoke the convolution theorem as follows:

$$\begin{aligned}\mathcal{F}\{f(t)\cos(2\pi at)\} &= F(f) * \frac{1}{2}\big(\delta(f+a) + \delta(f-a)\big) \\ &= \frac{1}{2}(F(f+a) + F(f-a))\end{aligned} \tag{114}$$

In other words, when we multiply a function, $f(t)$, by a cosine in direct space, we create two shifted copies of its Fourier transform, $F(f)$, in reciprocal space. It is possible for these shifted copies of $F(f)$ to overlap.

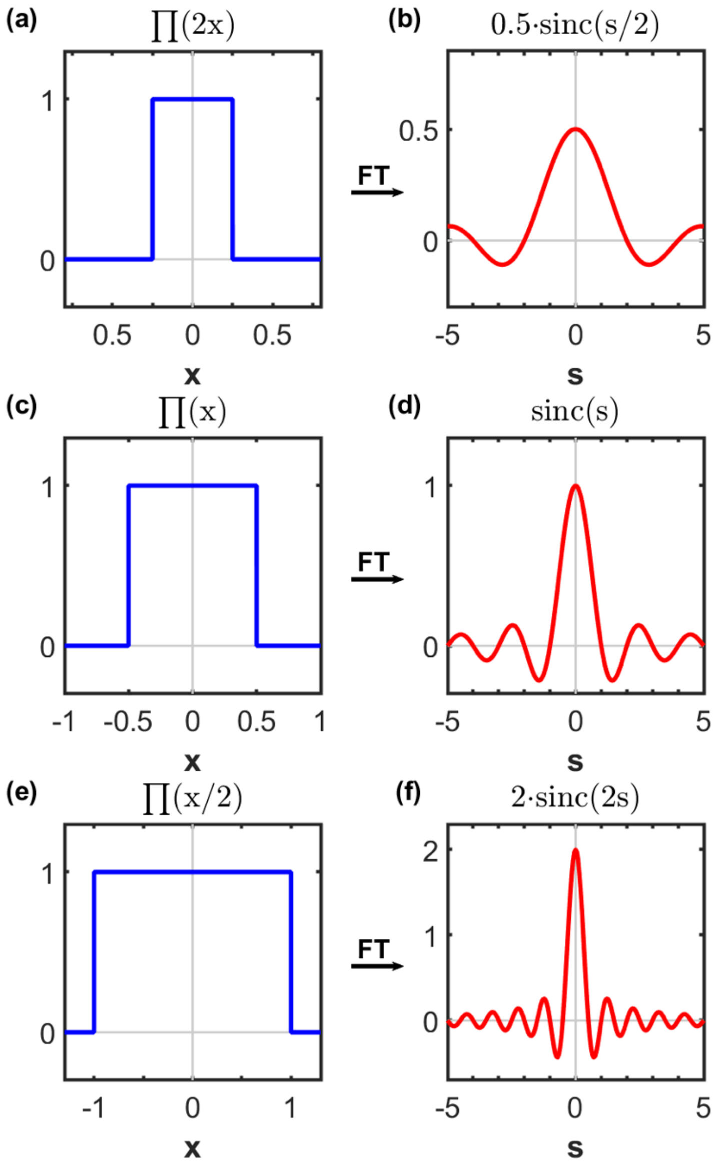

Figure 19. Illustration of the reciprocal nature of the Fourier transforms. On the left, three boxcar functions are becoming progressively broader, while, on the right, their Fourier transforms (sinc functions) are becoming progressively narrower.

2. Reciprocal relationship between the widths of functions and their Fourier transforms

A general principle that shows up all over Fourier analysis is that narrower functions in direct space have broader Fourier transforms, and vice versa. For example, the infinitely narrow delta function has an infinitely wide Fourier transform, i.e., $\delta(x) \leftrightarrow 1$. This same message is expressed in the similarity theorem (Equation 71), which reveals that contraction (squeezing) of a function in one domain leads to expansion of its Fourier transform (with scaling). Any time we have narrower or sharper features in a domain, we should anticipate that its corresponding Fourier transform will be broadened. As a graphical example of this, Figure 19 shows three boxcar functions with different widths and their corresponding Fourier transforms, which get narrower as the boxcar functions become wider. The basic idea here is that it requires many frequency/sinusoid components to recreate sharp features, but fewer to create narrower features. Furthermore, with regards to the boxcar $\leftrightarrow$ sinc Fourier pair, we notice that the boxcar function, which has a sharp cutoff, has a Fourier transform with values extending out to infinity. On the other hand, the sinc function, which is smooth, is made up of frequencies over only a finite range around the origin, and no others.

M. *Reversibility/reciprocity of the Fourier transform and the Fourier transform of the Fourier transform*

1. *Reversibility/reciprocity of the Fourier transform*

The Fourier transform is reversible. Accordingly, we expect to be able to substitute Equation 6, $F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx}dx$, into Equation 7, $f(x) = \int_{-\infty}^{\infty} F(s)e^{i2\pi sx}ds$, for $F(s)$ and get $f(x)$ back. To show this, we first recognize that x behaves differently in these equations. In Equation 6, it is a dummy variable that ranges from $-\infty$ to ∞, while in Equation 7 it refers to a specific value. Accordingly, we change the dummy variable x in Equation 6 to τ: $F(s) = \int_{-\infty}^{\infty} f(\tau)e^{-i2\pi s\tau}d\tau$ and substitute it into Equation 7 to give:

$$f(x) = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} f(\tau) e^{-i2\pi s\tau} d\tau \right] e^{i2\pi sx} ds \tag{115}$$

As is the case for a number of the proofs in this document, we now switch the order of integration, as follows:

$$f(x) = \int_{-\infty}^{\infty} f(\tau) \left[\int_{-\infty}^{\infty} e^{-i2\pi s\tau} e^{i2\pi sx} ds \right] d\tau \tag{116}$$

We now recall that the Fourier transform of a shifted delta function, $\delta(x - \tau)$, is $e^{-i2\pi s\tau}$, and the middle integral in Equation 116 is the inverse Fourier transform of $e^{-i2\pi s\tau}$, which means that this inner integral must be $\delta(x - \tau)$. Thus, Equation 116 becomes:

$$f(x) = \int_{-\infty}^{\infty} f(\tau)\delta(x - \tau) d\tau = f(x) \tag{117}$$

and our proof is complete.

2. *The Fourier transform of the Fourier transform*

When the Fourier transform was introduced, we saw that the kernels of the forward ($e^{-i2\pi sx}$) and reverse ($e^{i2\pi sx}$) transforms are not identical. We now ask what happens when we apply the forward transfer twice to a function. In other words, if $\mathcal{F}f(x) = F(s)$, which, again, we might write as $\mathcal{F}f = F$, what is $\mathcal{F}\mathcal{F}f$? To explore this problem, we note that $\mathcal{F}\mathcal{F}f = \mathcal{F}F$ and write:

$$\mathcal{F}\mathcal{F}f = \mathcal{F}F = \int_{-\infty}^{\infty} F(s)e^{-i2\pi sx}ds = \int_{-\infty}^{\infty} F(s)e^{i2\pi(-x)s}ds = f(-x) \tag{118}$$

So, applying the Fourier transform twice to a function, $f(x)$, produces $f(-x)$, not the original function. However, for an even function, $E(x)$, $E(-x) = E(x)$ so $\mathcal{F}\mathcal{F}E = E$. Using the methods outlined in this section, it can be shown that $\mathcal{F}\mathcal{F}\mathcal{F}\mathcal{F}f = f$.

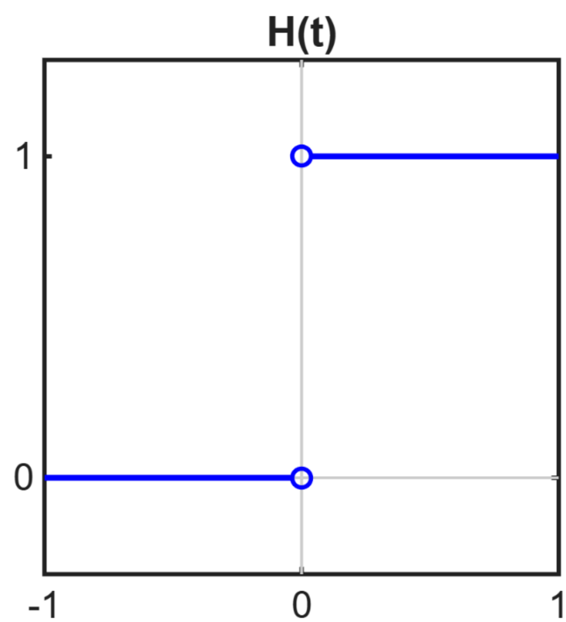

Figure 20. The Heaviside step function, $H(t)$, function as defined in Equation 119. In Equation 119, $H(t)$ is not defined at $t = 0$.

N. *Two other common functions in Fourier theory: the Heaviside step function and the signum or sign function*

1. The Heaviside step function

The Heaviside step function (see Figure 20), $H(t)$, is named for the great English engineer Oliver Heaviside, who was mathematically gifted. It is also sometimes referred to as the unit step function, $u(t)$. $H(t)$, or $u(t)$, is zero at $t < 0$ and unity for $t > 0$. That is:

$$H(t) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases} \tag{119}$$

Obviously, $H(t)$ can be defined differently at $t = 0$, where the resulting functions differ from each other by a null function. For example, one might define the function $H_a(t) = H(t) + \frac{1}{2}\delta^0(t)$ where:

$$H_a(t) = \begin{cases} 1 \; for \; x > 0 \\ \dfrac{1}{2} \; at \; x = 0 \\ 0 \; for \; x < 0 \end{cases} \tag{120}$$

When a function is multiplied by the Heaviside step function, $H(t)$ 'turns it on' at $t = 0$. Thus, $H(t)$ is used to guarantee that no 'action' takes place before $t = 0$.

The Heaviside step function can be obtained by integrating across the delta function as follows:

$$H_a(x) = \int_{-\infty}^{x} \delta(x')dx' \tag{121}$$

The Heaviside step function can be used in various functions and definitions. For example, one might define a ramp function, $R(x)$, with the properties:

$$R(x) = \begin{cases} x, & x > 0 \\ 0, & x < 0 \end{cases} \tag{122}$$

where $R(x)$ is also equal to:

$$R(x) = \int_{-\infty}^{x} H(x')dx' \tag{123}$$

In addition, $R(x) = H(x) * H(x)$.

The top hat function may be defined via $H(x)$ as $\Pi(x) = \frac{1}{2}\left(H\left(x + \frac{1}{2}\right) + H\left(-x + \frac{1}{2}\right)\right)$.

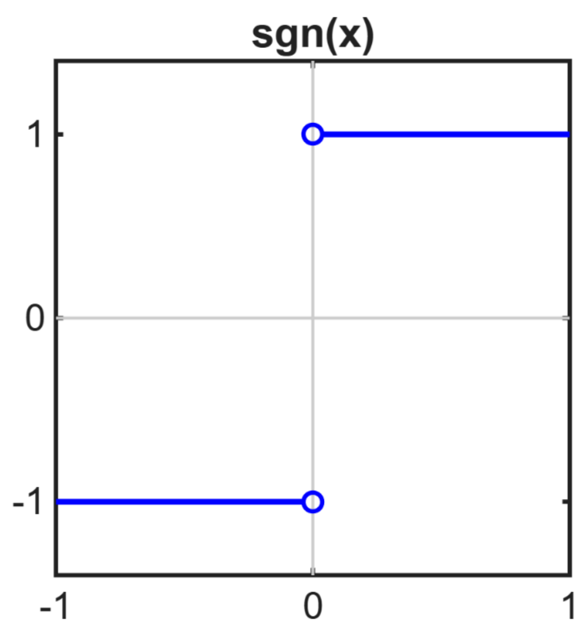

Figure 21. The signum, or sign function, $sgn(x)$, as defined in Equation 124.

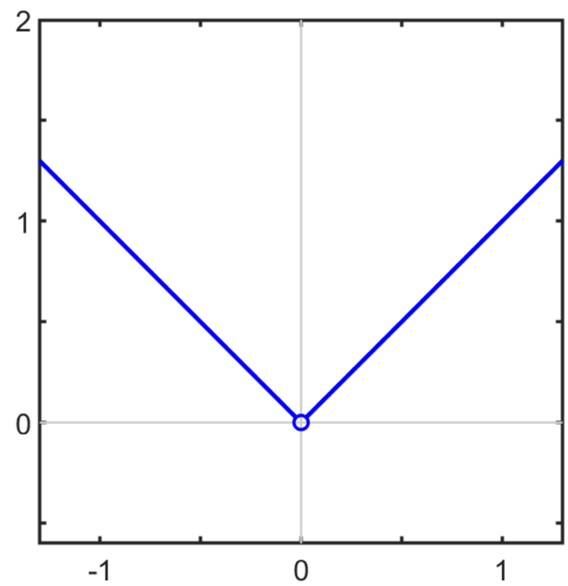

Figure 22. The function $x\ sgn(x)$.

2. The signum or sign function

The signum, or sign, function (see Figure 21), $sgn(x)$, is defined as:

$$sgn(x) = \begin{cases} 1, & x > 0 \\ -1, & x < 0 \end{cases} \tag{124}$$

Like the Heaviside step function, its definition at $x = 0$ can be left uncertain to within a null function. It can be defined in terms of the Heaviside step function as: $sgn(x) = 2H(x) - 1$.

As an example of its use, Figure 22 shows $x\ sgn(x)$, which has the shape of a 'v'.

As an additional example, in a problem in his book,[3] Bracewell asks the student to prove that $\Lambda'(x) = -\Pi\left(\frac{x}{2}\right) sgn(x)$, where $\Lambda'(x)$ is the derivative of the triangle function. This can be shown by rewriting $\Lambda(x)$ as:

$$\Lambda(x) = \begin{cases} 1 - x, 0 < x < 1 \\ 1 + x, -1 < x < 0 \\ 0, |x| > 1 \end{cases} \tag{125}$$

Thus:

$$\Lambda'(x) = \begin{cases} -1, 0 < x < 1 \\ 1, -1 < x < 0 \\ 0, \ \ |x| > 1 \end{cases} \tag{126}$$

To analyze the function $-\Pi\left(\frac{x}{2}\right) sgn(x)$, we first consider $\Pi\left(\frac{x}{2}\right)$. This function is:

$$\Pi\left(\frac{x}{2}\right) = \begin{cases} 1, -1 < x < 0 \\ 1, 0 < x < 1 \\ 0, \ \ |x| > 1 \end{cases} \tag{127}$$

Accordingly:

$$-\Pi\left(\frac{x}{2}\right) = \begin{cases} -1 \, for - 1 < x < 0 \\ -1 \, for \; 0 < x < 1 \\ 0, \ \ |x| > 1 \end{cases} \tag{128}$$

And finally:

$$-\Pi\left(\frac{x}{2}\right) sgn(x) = \begin{cases} 1 \, for - 1 < x < 0 \\ -1 \, for \; 0 < x < 1 \\ 0, \ \ |x| > 1 \end{cases} \tag{129}$$

Which shows that $\Lambda'(x) = -\Pi\left(\frac{x}{2}\right) sgn(x)$.

3. The Fourier transform of the signum function, $sgn(x)$

To find the Fourier transform of the signum function, $sgn(x)$, we consider a function that approaches $sgn(x)$ in a limit. One possible function is:

$$\lim_{a\to\infty} e^{\frac{-1}{a}|x|} sgn(x) \tag{130}$$

We now consider the Fourier transform of this function, break it into two integrals, combine terms, perform the integrations, and consider the limit as $a \to \infty$:

$$\lim_{a\to\infty} \int_{-\infty}^{\infty} e^{\frac{-1}{a}|x|}\, sgn(x)\, e^{-i2\pi sx} dx \tag{131}$$

$$= -\lim_{a\to\infty} \int_{-\infty}^{0} e^{\frac{1}{a}x} e^{-i2\pi sx} dx + \lim_{a\to\infty} \int_{0}^{\infty} e^{\frac{-1}{a}x}\, e^{-i2\pi sx}\, dx$$

$$= -\lim_{a\to\infty} \int_{-\infty}^{0} e^{\left(\frac{1}{a}-i2\pi s\right)x} dx$$

$$+ \lim_{a\to\infty} \int_{0}^{\infty} e^{\left(-\frac{1}{a}-i2\pi s\right)x} dx$$

$$= \lim_{a\to\infty} \left(\frac{-1}{\frac{1}{a} - i2\pi s} e^{\left(\frac{1}{a}-i2\pi s\right)x} |_{-\infty}^{0} \right)$$

$$+ \lim_{a\to\infty} \left(\frac{1}{-\frac{1}{a} - i2\pi s} e^{\left(-\frac{1}{a}-i2\pi s\right)x} |_{0}^{\infty} \right) = \lim_{a\to\infty} \frac{-1}{\frac{1}{a} - i2\pi s}$$

$$- \lim_{a\to\infty} \frac{1}{-\frac{1}{a} - i2\pi s} = \frac{-1}{-i2\pi s} + \frac{-1}{-i2\pi s} = \frac{1}{i\pi s}$$

This proof may seem like cheating, but it is not. For example, the $e^{\left(\frac{1}{a}-i2\pi s\right)x}$ term can be rewritten as $e^{\left(\frac{x}{a}\right)}e^{-i2\pi sx}$, where in $e^{\left(\frac{x}{a}\right)}$ we first let $x \rightarrow -\infty$ in applying the limits of the integral and then allow $a \rightarrow \infty$, which looks like $e^{\left(\frac{-\infty}{\infty}\right)}$. This approach is actually a standard trick for evaluating improper integrals. It simulates the fact that the infinite number of oscillations at infinity can be viewed as averaging to zero, which results in a reasonable way to simulate the real problem. That is, adding a function to force the integrand to vanish at large arguments is a way of simulating the cancellation that occurs anyway because the function is oscillating around zero and integrates to zero for any complete cycle. By including a decreasing exponential, we simulate this behavior with a function that actually does average to zero and approaches zero at large values of the integration variable.

4. The Fourier transform of the Heaviside step function, $H(x)$

Now that we have the Fourier transform of the sign or signum function, $\mathcal{F}(sgn(x)) = \frac{1}{i\pi s}$, we can easily obtain the Fourier transform of the Heaviside step function, where $H(x) = \frac{1}{2}(sgn(x) + 1)$. Thus:

$$\mathcal{F}\big(H(x)\big) = \mathcal{F}\left(\frac{1}{2}(sgn(x) + 1)\right) = \mathcal{F}\left(\frac{1}{2}sgn(x)\right) + \mathcal{F}\left(\frac{1}{2}\right) = \frac{1}{2i\pi s} + \frac{1}{2}\delta(s) \tag{132}$$

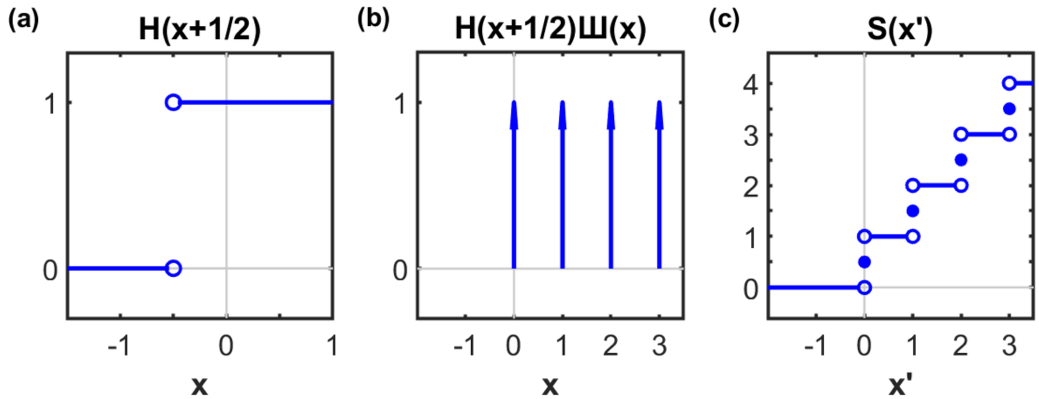

Figure 23. (a) The function $H\left(x+\frac{1}{2}\right)$, which is a shifted Heaviside step function, (b) The function $H\left(x+\frac{1}{2}\right)Ш(x)$, and (c) The integral $S(x')=\int_{-\infty}^{x'}H\left(x+\frac{1}{2}\right)Ш(x)dx$ for different values of x'. Note: the delta functions that the $Ш(x)$ function are based on are symmetric about each integer value where they are located. Accordingly, when we are exactly at an integer value in the integral for $x' \geq 0$, we have captured half the area of that delta function.

5. *An example problem that uses $H(x)$*

Plot $H\left(x+\frac{1}{2}\right)Ш(x)$ and $S(x')$, which are the integrand and function in Equation 133 (see answer/plots in Figure 23).

$$S(x')=\int_{-\infty}^{x'}H\left(x+\frac{1}{2}\right)Ш(x)dx \tag{133}$$

6. *A second example problem that uses two special functions*

The students in a Linford group meeting were recently presented with the following problem from Bracewell. When one of the students saw its solution, he exclaimed: "It's witchcraft!" It's actually not witchcraft. There's no such thing – see above. It's just the application of the ideas presented in this document. Show that for $\tau > 0$:

$$\lim_{\tau \to o} \int_{-\infty}^{\infty} -x\tau^{-2}\Pi\left(\frac{x}{2\tau}\right) sgn(x)\, dx = -1 \tag{134}$$

To solve this problem, we first recognize that the $\Pi(x)$ function is only non-zero where its argument ranges from $-\frac{1}{2}$ to $\frac{1}{2}$, which corresponds to $\frac{x}{2\tau} = \frac{-1}{2}$ and $\frac{x}{2\tau} = \frac{1}{2}$ or $x = -\tau$ to $x = \tau$, and also that τ^{-2} is a constant in the integral. Accordingly, we can change our integral to:

$$\lim_{\tau \to o} \tau^{-2} \int_{-\tau}^{\tau} -x\, sgn(x)\, dx \tag{135}$$

We next recognize that both x and $sgn(x)$ are odd, so their product is even, so:

$$2 \lim_{\tau \to o} \tau^{-2} \int_{0}^{\tau} -x\, sgn(x)\, dx \tag{136}$$

Next, we observe that $sgn(x)$ is unity from 0 to τ, so we can remove this function from the integral to obtain:

$$2 \lim_{\tau \to o} \tau^{-2} \int_{0}^{\tau} -x\, dx \tag{137}$$

Moving the minus sign out of the integral, performing this trivial integral, and inserting the limits gives:

$$-2 \lim_{\tau \to o} \tau^{-2} \frac{\tau^2}{2} \tag{138}$$

Thus, τ and 2 cancel out of the equation, the $\lim_{\tau \to o}$ term turns out to be unnecessary, and we are left with the desired result of -1.

O. *Limitations of the Fourier transform*

The Fourier theory described so far in this article is powerful and rich. It is of great theoretical importance. It provides a strong foundation for understanding other aspects of Fourier theory. However, it is of limited practical value because of the difficulty associated with determining the Fourier transforms (integrals) associated with many functions. An additional challenge is that real data, e.g., spectra, are usually discrete, so Equation 6 cannot be used with them. In the next part of this article, we discuss the discrete Fourier transform, which provides a way to calculate the Fourier transforms of discrete data.

VII. The Discrete Fourier Transform (DFT)

A. *Sequences of numbers and their arithmetic*

1. Sequences of numbers

The discrete Fourier transform (DFT) deals with sequences of numbers, not continuous functions. Unlike in a set, where the order of the numbers does not matter, the order of the numbers in a sequence does matter. The DFT also deals with finite, not infinite, sequences, where, in general, the numbers in them are evenly spaced. For example, in a spectrum we might have a number of counts, $Counts_i$, at a series of evenly spaced energies, E_i, where we might write this spectrum as a sequence of N ordered pairs, as follows: $\{(E_1, Counts_1), (E_2, Counts_2), \dots, (E_N, Counts_N)\}$. However, for the DFT, we will generally use abbreviated sequences like: $\{x_0, x_1, \dots, x_{N-1}\}$ to represent spectra, which are indexed to start with a zeroth element, x_0. We might also represent these sequences as $\{x_i\}_{i=0}^{N-1}$, $\{x_i\}$, or even just x_i.

2. *The Arithmetic of Sequences*

As a quick reminder, when sequences are added, subtracted, multiplied, or divided, corresponding entries in the sequences are added, subtracted, multiplied, or divided, respectively.

For example, consider the following two sequences: $\{x_i\} = \{1, i, 4, -3\}$ and $\{y_i\} = \{6, 2 + i, -5, 17\}$.

$$\{x_i\} + \{y_i\} = \{1 + 6, i + 2 + i, 4 - 5, -3 + 17\} = \{7, 2 + 2i, -1, 14\} \tag{139}$$

$$\{x_i\} - \{y_i\} = \{1 - 6, i - 2 - i, 4 + 5, -3 - 17\} = \{-5, -2, 9, -20\} \tag{140}$$

$$\{x_i\}\{y_i\} = \{1 \cdot 6, i \cdot (2 + i), 4 \cdot (-5), -3 \cdot 17\} = \{6, -1 + 2i, -20, -51\} \tag{141}$$

$$\frac{\{x_i\}}{\{y_i\}} = \left\{\frac{1}{6}, \frac{i}{2+i}, \frac{4}{-5}, \frac{-3}{17}\right\} = \left\{\frac{1}{6}, \frac{1+2i}{5}, \frac{-4}{5}, \frac{-3}{17}\right\} \tag{142}$$

Of course, division of sequences, e.g., Equation 142, assumes that no y_i is zero.

Finally, when we multiply a sequence, e.g., $\{x_i\}$, by a constant, a, we get:

$$a\,\{x_i\} = a\,\{1, i, 4, -3\} = \{a, ia, 4a, -3a\} \tag{143}$$

B. *Definition of the DFT (as a Sum), and a Disclaimer*

1. *Definition of the Discrete Fourier Transform (DFT)*

The Fourier transform and inverse Fourier transform of continuous functions (Equations 6 and 7) are based on integrals. In contrast, the DFT and inverse DFT given in Equations 144 and 145 are based on sums, as follows:

$$C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} \tag{144}$$

$$x_n = \frac{1}{N}\sum_{k=0}^{N-1} C_k e^{i2\pi n(k/N)} \tag{145}$$

Some authors, including Bracewell[3] and Weaver,[9] place the $\frac{1}{N}$ normalization term before the sum in Equation 144 instead of as it is in this work in Equation 145. However, the DFT as defined in

Equations 144 and 145 appears to be the more common way of defining currently. MATLAB uses these versions for its 'fft' and 'ifft' commands as do Walker[12] and Leis.[14] Of course, if the DFT is defined as $C_k = \frac{1}{N}\sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)}$ then C_0 is just the average of the entries in $\{x_n\}$. For us, in Equation 144, C_0 is the sum of the entries in $\{x_n\}$.

Obviously, we can expand Equations 144 and 145 using Euler's relationship as follows:

$$C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} = \sum_{n=0}^{N-1} x_n(\cos\big(2\pi k(n/N)\big) - isin(2\pi k(n/N))) \tag{146}$$

$$x_n = \frac{1}{N}\sum_{k=0}^{N-1} C_k e^{i2\pi n(k/N)} = \frac{1}{N}\sum_{k=0}^{N-1} C_k(\cos\big(2\pi k(n/N)\big) + isin(2\pi k(n/N))) \tag{147}$$

It might be assumed that because Equations 6 and 9 are based on more advanced mathematics (integrals compared to sums) than Equations 144 and 145, Equations 6 and 9 (and other integrals like them in Fourier theory) would be, in general, harder to understand. This is not always the case. David Aspnes has observed: "People understand integrals; they don't understand sums." Accordingly, to help people become more familiar and comfortable with the DFT, this tutorial contains multiple examples of using the DFT. In general, these examples are presented as problems. Those new to DFTs will probably learn this material better by working them than by simply looking at their solutions.

2. Disclaimer

As was the case above with the Fourier transform above, we will only consider the DFT of real sequences of numbers. Of course, there is no reason, mathematically, not to apply the DFT to sequences of complex numbers. We focus on sequences of real numbers because the spectra we are interested in denoising are real.

C. *Viewing the DFT as an extension of the Fourier transform of continuous functions*

There are several ways to understand the DFT and inverse DFT. However, no matter how we consider them, the DFT and inverse DFT transform finite sequences of numbers into finite sequences of numbers of the same length, which may be complex.

The DFT can be defined via the sums in Equations 144 and 145, which will be considered in detail in the next sections. It can also be viewed as a matrix algebra problem.[13] Furthermore, it is sometimes justified as an extension of the Fourier transforms of continuous functions, as follows. Consider a continuous function, $f(x)$, and its Fourier transform, $F(s)$. To discretize $f(x)$, it is multiplied by a shah function, e.g., $Ш(x)$ (see above), to produce $f(x)Ш(x)$, which replaces $f(x)$ with a series of evenly spaced delta functions that have the values of $f(x)$ where the delta functions are located. A consequence of this action in direct space is the replication of $F(s)$ an infinite number of times through the convolution $F(s) * Ш(s)$ in reciprocal space (recall that $Ш(x) \leftrightarrow Ш(s)$). Some overlap, known as aliasing, between the copies of $F(s)$ may take place in this process. Obviously, this convolution works best, and is simplest, if $F(s)$ is bandlimited, which means that $F(s)$ is zero beyond a cutoff value. More specifically, if $F(s)$ is bandlimited, we will want to sample $f(x)$ with delta functions that are closely enough spaced so that the corresponding delta functions in the shah function in reciprocal space are far enough apart that the copies of $F(s)$

do not overlap. In other words, the choice of $Ш(x) \leftrightarrow Ш(s)$ suggested in this paragraph may not be the right one.

Now that the data are discretized in real space, we repeat this process, but starting from reciprocal space. That is, one multiplies the replicated function based on $F(s)$ in reciprocal space by a shah function, which discretizes the function in reciprocal space. Through the convolution theorem, this process replicates the already discretized function in direct space. Through this process, one ends up with discrete, periodic data in both domains. These arguments provide some insight into and justification for the idea of the DFT as an extension of the Fourier transform.

D. *The Discrete Fourier Transform as a Sum*

We now explore Equations 144 and 145, which provide a definition of the DFT based on sums. At this point, we aren't concerned how we got the definitions in Equations 144 and 145. We'll provide a deeper justification for them later.

We begin by pointing out some similarities between Equations 6 and 7 and Equations 144 and 145. An obvious one is the $e^{-i2\pi sx}$ and $e^{i2\pi sx}$ terms in Equations 6 and 7, respectively, and the $e^{-i2\pi nk/N}$ and $e^{i2\pi nk/N}$ terms in Equations 144 and 145, respectively. Both the Fourier transform and DFT have complex exponential terms, where, in each case, the forward transform has a minus sign and the reverse transform does not. Per Euler's relationship, all of these terms are ultimately sinusoidal. In particular, we can expand $e^{-i2\pi nk/N}$ and $e^{i2\pi nk/N}$ (the kernels of the DFT) as:

$$e^{-i2\pi k(n/N)} = cos\left(2\pi k\left(\frac{n}{N}\right)\right) - i\,sin\left(2\pi k\left(\frac{n}{N}\right)\right) \tag{148}$$

$$e^{i2\pi k(n/N)} = cos\left(2\pi k\left(\frac{n}{N}\right)\right) + i\,sin\left(2\pi k\left(\frac{n}{N}\right)\right) \tag{149}$$

From Equations 6 and 7, it is clear that in the forward and reverse Fourier transforms we multiply two functions together and take their integral, where one of these functions is a sinusoid of varying frequency. While it may not be quite as obvious in Equations 144 and 145 what is going on, it is basically the same thing. In Equations 144 and 145, a sequence of data points represented as x_n and C_k, respectively, is multiplied by another sequence of data points obtained from $e^{-i2\pi k(n/N)}$ and $e^{i2\pi k(n/N)}$, which, per Euler's relationship, are taken across cosine and sine functions with different frequencies. However, a key difference between the Fourier transform and the DFT is the nature of these frequences. In Equation 6, $F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx}dx$, s, which is the frequency in $e^{-i2\pi sx}$, takes on all possible values. In contrast, in Equation 144, $C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)}$, k, which is the frequency in $e^{-i2\pi k(n/N)}$, is an integer that takes on values from 0 to $N-1$. Indeed, k gives the number of cycles of the sines and cosines in $e^{-i2\pi k(n/N)}$ through Euler's formula that fit and are sampled between $n = 0$ and $n = N-1$.

In the DFT (Equation 144), we multiply a sequence of N data points, which we specify as: x_0, x_1, x_2, …, x_{N-1}, by an equally long sequence of values obtained by considering $n = 0, 1, 2, \ldots, N-1$ in $e^{-i2\pi k(n/N)}$ for a given value of k and sum the resulting values. This process creates a different Fourier coefficient, C_k, for each value of k. The inverse DFT, Equation 145, is doing something very similar. In Equation 145, the sequence of Fourier coefficients

$\{C_0, C_1, \dots, C_{N-1}\}$ is multiplied by a sequence obtained by considering k from 0 to $N-1$ in $e^{i2\pi n(k/N)}$, where n is the sample index used in the underlying sinusoids.

Some who are new to the DFT have imagined that there is somehow a one-to-one correspondence or relationship between the individual numbers in the sequence of data points and the individual Fourier coefficients obtained from them. For example, they have thought that somehow x_0 is transformed into C_0, x_1 is transformed into C_1, etc. This is not the case. As just discussed and illustrated in the examples below, in the DFT all the data points in the original sequence are used to calculate each of the Fourier coefficients. Similarly, in the inverse DFT, all of the Fourier coefficients are used to recalculate each number in the original sequence.

Finally, note how we have written (n/N) in $e^{-i2\pi k(n/N)}$ (Equation 144). This is to emphasize that when we put $n = 0, 1, 2, \dots, N-1$ into $e^{-i2\pi k(n/N)}$ for a given value of k, (n/N) ranges from 0 to $\frac{N-1}{N}$, where $\frac{N-1}{N}$ approaches unity for large N. Again, in the DFT we are sampling across k waves/cycles over the N samples. The same thing is occurring in the inverse DFT (Equation 145) with $\frac{k}{N}$ and n.

E. *Examples of Applying the DFT to sequences of numbers*

Here are some examples of applying the DFT to real data and also the use of the inverse DFT.

Example 1. Take the DFT of {0, 1}.

Solution 1. For this problem, $N = 2$. Accordingly, we calculate C_0 and C_1, i.e., for $k = \{0, 1\}$, as follows:

$$C_k = C_0 = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} = \sum_{n=0}^{1} x_n e^{-i2\pi 0(n/2)} = \sum_{n=0}^{1} x_n = 0e^0 + 1e^0 = 1 \tag{150}$$

$$C_1 = \sum_{n=0}^{1} x_n e^{-i2\pi 1(n/2)} = \sum_{n=0}^{1} x_n e^{-i\pi n} = x_0 e^0 + x_1 e^{-i\pi} = 0 - 1 = -1 \tag{151}$$

So the DFT of {0, 1} to {1, -1}

Example 2. Calculate the DFT of a longer sequence of numbers: {1, 2, 3, 1}.

Solution 2. Now, $N = 4$, so we need to calculate four Fourier coefficients:

$$\begin{aligned} C_0 &= \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} \\ &= \sum_{n=0}^{3} x_n e^{-i2\pi 0(n/4)} = x_0 e^{-i2\pi 0(0/4)} + x_1 e^{-i2\pi 0(1/4)} \\ &+ x_2 e^{-i2\pi 0(2/4)} + x_3 e^{-i2\pi 0(3/4)} = x_0 + x_1 + x_2 + x_3 \\ &= 1 + 2 + 3 + 1 = 7 \end{aligned} \tag{152}$$

$$\begin{aligned} C_1 &= \sum_{n=0}^{3} x_n e^{-i2\pi 1(n/4)} \\ &= x_0 e^{-i2\pi 1(0/4)} + x_1 e^{-i2\pi 1(1/4)} + x_2 e^{-i2\pi 1(2/4)} + x_3 e^{-i2\pi 1(3/4)} \\ &= x_0 e^0 + x_1 e^{-i\pi/2} + x_2 e^{-i\pi} + x_3 e^{-i3\pi/2} = 1 - 2i - 3 + i \\ &= -2 - i \end{aligned} \tag{153}$$

$$C_2 = \sum_{n=0}^{3} x_n e^{-i2\pi 2(n/4)} = \sum_{n=0}^{3} x_n e^{-i\pi n} = 1 - 2 + 3 - 1 = 1 \tag{154}$$

$$C_3 = \sum_{n=0}^{3} x_n e^{-i2\pi 3(n/4)} = \sum_{n=0}^{3} x_n e^{-i\pi n3/2} = 1 + 2i - 3 - i = -2 + i \tag{155}$$

Thus, the discrete Fourier transform of {1, 2, 3, 1} is {7, $-2 - i$, 1, $-2 + i$ }. Notice that two of these coefficients are complex.

Example 3. Calculate the DFT of {1, 1, 1, 1}, which is the discrete analog of $f(x) = 1$. Weaver refers to {1, 1, 1, 1} as the unit constant sequence.[9]

Solution 3. For $N = 4$ we obtain

$$C_0 = \sum_{n=0}^{3} x_n e^{-i2\pi 0(n/4)} = 1 \cdot e^0 + 1 \cdot e^0 + 1 \cdot e^0 + 1 \cdot e^0 = 4 \tag{156}$$

$$\begin{aligned} C_1 &= \sum_{n=0}^{3} x_n e^{-i2\pi 1(n/4)} = 1 \cdot e^0 + 1 \cdot e^{-i\pi/2} + 1 \cdot e^{-i\pi} + 1 \cdot e^{-i3\pi/2} \\ &= 1 - i - 1 + i = 0 \end{aligned} \tag{157}$$

$$C_2 = \sum_{n=0}^{3} x_n e^{-i\pi n} = 1 - 1 + 1 - 1 = 0 \tag{158}$$

$$C_3 = \sum_{n=0}^{3} x_n e^{-i2\pi 3(n/4)} \sum_{n=0}^{3} x_n e^{-i\pi n3/2} = 1 + i - 1 - i = 0 \tag{159}$$

Thus, the discrete Fourier transform of $\{1, 1, 1, 1\}$ is $\{4, 0, 0, 0\}$, which is the discrete analog of the delta function, the so-called 'delta sequence': $\{1, 0, 0, 0\}$, multiplied by 4. This result is not a coincidence.

Example 4. Calculate the DFT of the delta sequence, $\{1, 0, 0, 0\}$.

Solution 4. For $N = 4$ we obtain

$$C_0 = \sum_{n=0}^{3} x_n e^{-i2\pi 0(n/4)} = 1 + 0 + 0 + 0 = 1 \tag{160}$$

$$C_1 = \sum_{n=0}^{3} x_n e^{-i2\pi 1(n/4)} = 1 + 0 + 0 + 0 = 1 \tag{161}$$

$$C_2 = \sum_{n=0}^{3} x_n e^{-i2\pi 2(n/4)} = 1 + 0 + 0 + 0 = 1 \tag{162}$$

$$C_3 = \sum_{n=0}^{3} x_n e^{-i2\pi 3(n/4)} = 1 + 0 + 0 + 0 = 1 \tag{163}$$

Again, this DFT transform pair, $\{1, 0, 0, 0\} \leftrightarrow \{1, 1, 1, 1\}$, is closely related to what we obtained in our study of the Fourier transforms of continuous functions. This is not coincidental.

Example 5. Show that any delta sequence of length, N, is a unit constant sequence of the same length. That is, if $\{x_i\}_{i=0}^{N-1} = \{1, 0, 0, \dots, 0\}$, its DFT is $\{C_k\}_{i=0}^{N-1} = \{1, 1, 1, \dots, 1\}$.

Solution 5. We go back to the definition of the DFT: $C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)}$ and recognize that because $\{x_i\}_{i=0}^{N-1} = \{1, 0, 0, \dots, 0\}$, only the first term of this series survives (all the rest are zero). Thus, $C_k = x_0 e^{-i2\pi k(0/N)} = x_0 = 1$, i.e., all the C_k are unity, which completes our proof.

Example 6. Now let's confirm that the inverse DFT returns the sequence we started with in Example 1, where we were asked to calculate the DFT of {0, 1}, which we found to be {1, -1}.

Solution 6. For $N = 2$ and {1, -1} in the inverse DFT we obtain:

$$x_n = x_0 = \frac{1}{N}\sum_{k=0}^{N-1} C_k e^{i2\pi n(k/N)} \tag{164}$$

$$= \frac{1}{2}\sum_{k=0}^{1} C_k e^{i2\pi 0k/2} = 1 \cdot e^0 + (-1) \cdot e^0 = 1 - 1 = 0$$

$$x_1 = \frac{1}{2}\sum_{k=0}^{1} C_k e^{i2\pi 1k/2} = \frac{1}{2}\left(1 \cdot e^0 + (-1) \cdot e^{i\pi}\right) = 1 \tag{165}$$

That is, as expected, the inverse DFT of {1, -1} is {0, 1}.

Example 7. In Example 2 above, we found that the DFT of $x_n = \{1, 2, 3, 1\}$ is $C_k = \{7, -2 - i, 1, -2 + i\}$. Let's check this result by taking the inverse DFT of {7, $-2 - i$, 1, $-2 + i$ }.

Solution 6. For $N = 4$ and $\{7, -2-i, 1, -2+i\}$ in Equation 145 we obtain:

$$x_0 = \frac{1}{4}\sum_{k=0}^{3} C_k e^{i2\pi 0(k/4)} = \frac{1}{4}(7 \cdot e^0 + (-2-i) \cdot e^0 + 1 \cdot e^0 + (-2+i) \cdot e^0) = 1 \tag{166}$$

$$\begin{aligned} x_1 &= \frac{1}{4}\sum_{k=0}^{3} C_k e^{i2\pi 1(k/4)} \\ &= \frac{1}{4}\left(7 \cdot e^{i2\pi 1(0/4)} + (-2-i) \cdot e^{i2\pi 1(1/4)} + 1 \cdot e^{i2\pi 1(2/4)} + (-2 + i) \cdot e^{i2\pi 1(3/4)}\right) \\ &= \frac{1}{4}\left(7e^0 + (-2-i)e^{i\pi/2} + 1e^{i\pi} + (-2+i)e^{i\pi(3/2)}\right) \\ &= \frac{1}{4}\left(7 + (-2-i) \cdot i - 1 + (-2+i) \cdot (-i)\right) \\ &= \frac{1}{4}(7 - 2i + 1 - 1 + 2i + 1) = 2 \end{aligned} \tag{167}$$

$$\begin{aligned} x_2 &= \frac{1}{4}\sum_{k=0}^{3} C_k e^{i2\pi 2(k/4)} \\ &= \frac{1}{4}\left(7 \cdot e^{0\pi} + (-2-i) \cdot e^{i\pi} + 1 \cdot e^{i2\pi} + (-2+i) \cdot e^{i3\pi}\right) \\ &= \frac{1}{4}\left(7 + (-2-i)(-1) + 1 \cdot 1 + (-2+i) \cdot (-1)\right) = 3 \end{aligned} \tag{168}$$

$$x_3 = \frac{1}{4}\sum_{k=0}^{3} C_k e^{i2\pi 3(k/4)} \tag{169}$$

$$= \frac{1}{4}\left(7 \cdot e^0 + (-2-i) \cdot e^{i\pi(3/2)} + 1 \cdot e^{i3\pi} + (-2+i) \cdot e^{i\pi(9/2)}\right)$$

$$= \frac{1}{4}(7 + (-2-i) \cdot (-i) + 1 \cdot (-1) + (-2+i) \cdot i) = 1$$

F. *Examples of sampled sines and cosines used in the DFT*

As mentioned above, only the sinusoids that fit into the length of the number of data points in the sequence of interest are employed in the DFT. We will now list or show a few sampled cosines and sines that could be used in a DFT. We will first do this for $N = 8$ to focus on the math and then for $N = 32$ to show some sampled waves. We will begin by using Euler's relationship to break Equation 144 into its real and imaginary parts.

$$C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} = \sum_{n=0}^{N-1} x_n \, cos\left(2\pi k\left(\frac{n}{N}\right)\right) - i\sum_{n=0}^{N-1} x_n \, sin\left(2\pi k\left(\frac{n}{N}\right)\right) \tag{170}$$

As an example, we now write out Equation 170 in Equation 171 for an arbitrary value of k and $N = 8$. That is, Equation 171 shows results for $\frac{n}{N} = \frac{n}{8}$ for $n = 0, 1 \ldots 7$. Equation 171 is a sampling at equal intervals across sines and cosines with frequencies k.

$$C_k = x_0\, cos\left(2\pi k\left(\frac{0}{8}\right)\right) + x_1\, cos\left(2\pi k\left(\frac{1}{8}\right)\right) + x_2\, cos\left(2\pi k\left(\frac{2}{8}\right)\right)$$
$$+ x_3\, cos\left(2\pi k\left(\frac{3}{8}\right)\right) + x_4\, cos\left(2\pi k\left(\frac{4}{8}\right)\right) + x_5\, cos\left(2\pi k\left(\frac{5}{8}\right)\right)$$
$$+ x_6\, cos\left(2\pi k\left(\frac{6}{8}\right)\right)$$
$$+ x_7\, cos\left(2\pi k\left(\frac{7}{8}\right)\right)$$
$$- i\left(x_0\, sin\left(2\pi k\left(\frac{0}{8}\right)\right) + x_1\, sin\left(2\pi k\left(\frac{1}{8}\right)\right) + x_2\, sin\left(2\pi k\left(\frac{2}{8}\right)\right)\right.$$
$$+ x_3\, sin\left(2\pi k\left(\frac{3}{8}\right)\right) + x_4\, sin\left(2\pi k\left(\frac{4}{8}\right)\right) + x_5\, sin\left(2\pi k\left(\frac{5}{8}\right)\right)$$
$$\left.+ x_6\, sin\left(2\pi k\left(\frac{6}{8}\right)\right) + x_7\, sin\left(2\pi k\left(\frac{7}{8}\right)\right)\right) \tag{171}$$

Now, for $N = 32$, Figure 24 - Figure 26 show the sampled sine and cosine waves produced in the DFT for $k = 0, 1,$ and 2. That is, these sampled waves will be multiplied by a sequence of 32 data points to produce C_0, C_1, and C_2 in a DFT. Thus, we see that the lower-index Fourier coefficients, C_k, are the result of multiplications of our sequence of numbers by lower frequency waves, and, as should be apparent, the higher Frequency coefficients are the result of multiplications of our sequence by higher frequency waves. Therefore, for discrete spectra that contain high frequency noise on broader peaks, the broader peaks and noise will be described by the lower-index and higher-index Fourier coefficients, respectively.

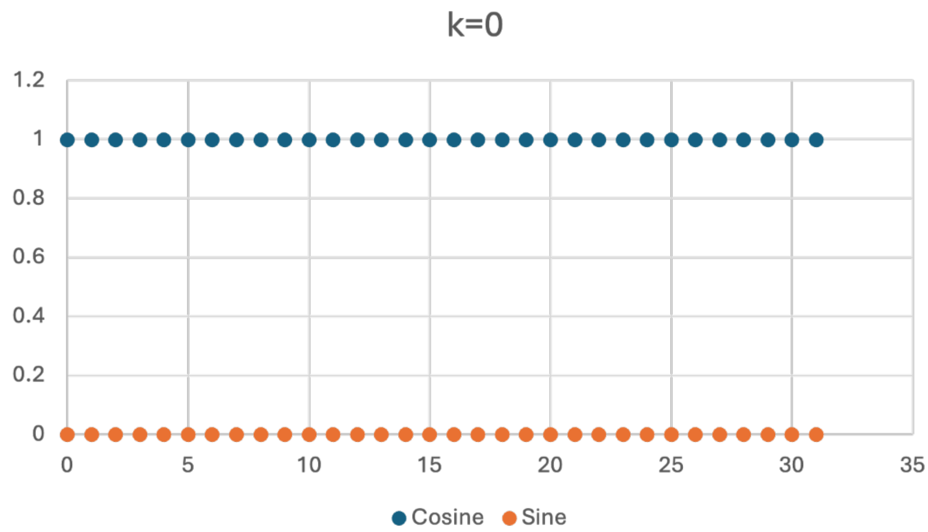

Figure 24. The cosine and sine 'waves' with $k = 0$ that are multiplied by a sequence of 32 data points ($N = 32$) in a DFT to produce C_0 as described in Equation 170.

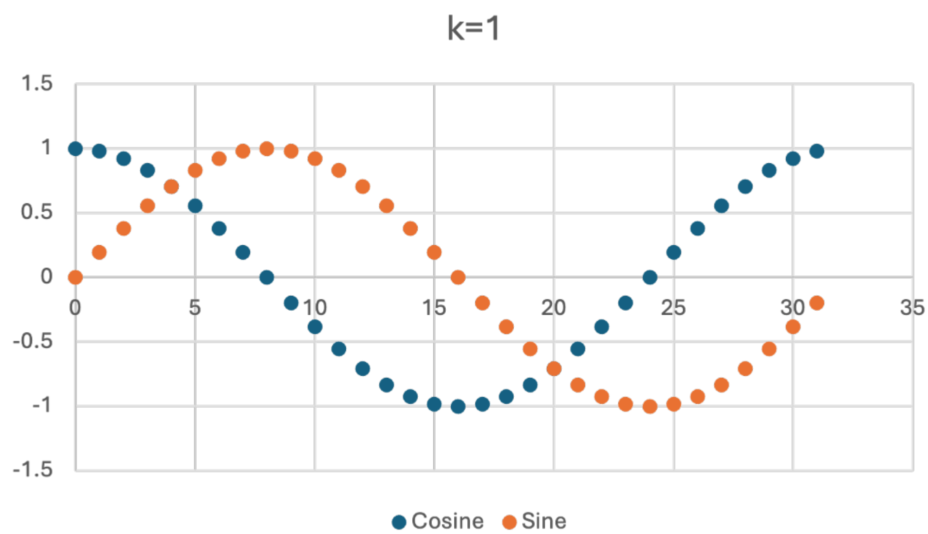

Figure 25. The cosine and sine waves with $k = 1$ that are multiplied by a sequence of 32 data points ($N = 32$) in a DFT to produce C_1 as described in Equation 170.

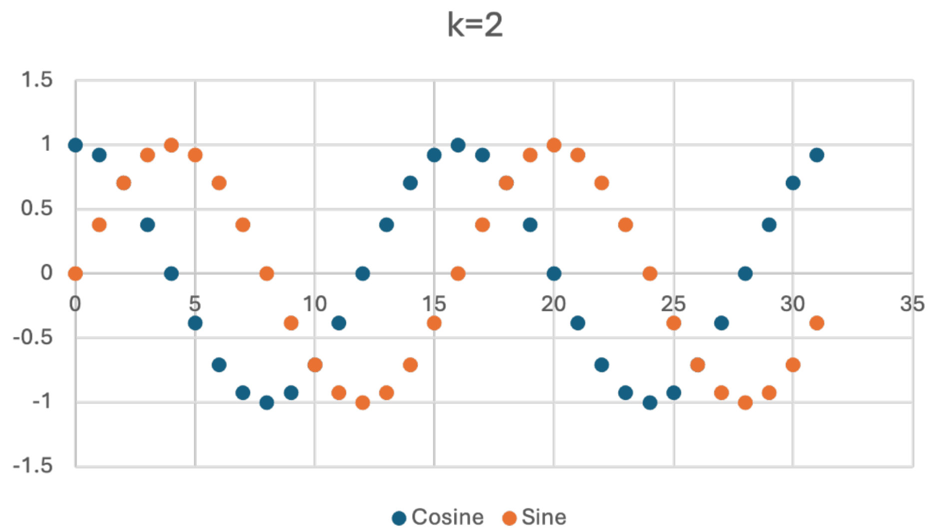

Figure 26. The cosine and sine waves with $k = 2$ that are multiplied by a sequence of 32 data points ($N = 32$) in a DFT to produce C_2 as described in Equation 170.

G. *The DFT and the inverse DFT are Periodic*

1. *The periodicity of the DFT and inverse DFT*

The DFT and inverse DFT are periodic in the number of data points N in the sequence. We can see this by considering C_{k+N} in Equation 144:

$$C_{k+N} = \sum_{n=0}^{N-1} x_n e^{-i2\pi(k+N)(n/N)}$$
$$= \sum_{n=0}^{N-1} x_n e^{-i2\pi(kn/N)} e^{-i2\pi n} = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} = C_k \tag{172}$$

Equation 172 is valid because n is an integer in $e^{-i2\pi n}$. Furthermore, even though spectra from analytical instruments are not infinitely periodic – they are not usually periodic in any way, they turn out to be periodic when we consider $x_n = x_{n+N}$, as follows, which again holds because k is an integer in $e^{i2\pi k}$:

$$x_{n+N} = \frac{1}{N}\sum_{k=0}^{N-1} C_k e^{i2\pi(n+N)(k/N)} = \frac{1}{N}\sum_{k=0}^{N-1} C_k e^{i2\pi n(k/N)} e^{i2\pi k} \tag{173}$$

$$= \frac{1}{N}\sum_{k=0}^{N-1} C_k e^{i2\pi n(k/N)} = x_n$$

2. *Even and odd sequences, an idea that uses the periodicity of the DFT*

As noted above, even and odd functions play an important role in the Fourier transform. It turns out that there are also even and odd sequences. Similar to what we saw for functions, a sequence, $\{x_i\}_{i=0}^{N-1}$, is even if $x_i = x_{-i}$ and odd if $x_i = -x_{-i}$. In these definitions, we invoke the periodicity of the sequences in the DFT and inverse DFT. For example, the following sequence with $N = 7$ is even: $\{2, -3, 4, 5, 5, 4, -3\}$. To show the evenness of this sequence, we rewrite it showing part of its periodicity: …, 2, −3, 4, 5, 5, 4, −3, **2**, −3, 4, 5, 5, 4, −3 …, where x_0, which is 2, is bolded and underlined. We note that $x_1 = x_{-1} = -3$, where because of the periodicity of the DFT, $x_1 = x_{N-1} = x_6 = -3$. Similarly, $x_2 = x_{-2} = 4$, where, again, because of the periodicity of the DFT, $x_2 = x_{N-2} = x_4 = 4$, etc. The first element, x_0, in an even sequence can have any value because, for $i = 0$, it will always satisfy $x_i = x_{-i} = x_0$.

The following sequence is odd: $\{0, -3, 4, 5, -5, -4, 3\}$. Note that the first element, x_0, in an odd sequence must be zero. It cannot have any value as is the case for even sequences. Rather, $x_0 = 0$ for odd sequences because for $i = 0$, $x_0 = -x_0$, which is only true if $x_0 = 0$. To help show the oddness of {0, −3, 4, 5, -5, -4, 3} we note that $x_1 = -x_{-1} = -x_{N-1} = -x_6 = -3$, $x_2 = -x_{-2} = -x_{N-2} = -x_5 = 4$, etc.

H. *The Weighting Kernel Abbreviates how the DFT is written*

The exponential terms, e.g., $e^{i2\pi(n+N)(k/N)}$, in the DFT equations above are fairly long to write out. Accordingly, they are often abbreviated and rewritten using the so-called weighting kernel, W_N. However, authors differ a little in how they define this kernel. Weaver defines it as $e^{i2\pi/N}$,[9] and Bagchi and Mitra define it as $e^{-i2\pi/N}$.[18] Of course, N is the number of data points in the sequence in W_N. Walker defines W_N to be both $e^{-i2\pi/N}$ and $e^{i2\pi/N}$, where he states that the context of its use should indicate which one is meant.[12] We will use $W_N = e^{-i2\pi/N}$ in this work. Certainly, in some calculations, it does not matter which version of W_N is used. For example, if we define $W_N^- = e^{-i2\pi/N}$ and $W_N^+ = e^{i2\pi/N}$, we see that for k an integer: $(W_N^-)^{Nk} = (W_N^+)^{Nk} = 1$.

Using the weighting kernel, we can rewrite the definitions of the forward and inverse DFT more tersely as:

$$C_k = \sum_{n=0}^{N-1} x_n W_N^{nk} \tag{174}$$

$$x_n = \frac{1}{N}\sum_{k=0}^{N-1} C_k W_N^{-nk} \tag{175}$$

I. *Confirming the Reversibility of the DFT Equation*

1. *The sum of a finite geometric series*

To perform the proof in the second part of this section, we will need the equation for the sum of a finite geometric series. To derive this sum, where this derivation is well-known, we consider the following two geometric series,

$$S = 1 + r + r^2 + \cdots + r^{N-1} \tag{176}$$

$$rS = r + r^2 + r^3 + \cdots + r^N \tag{177}$$

We now subtract rS from S to obtain:

$$S - rS = S(1 - r) = 1 - r^N \tag{178}$$

Solving for S gives us:

$$S = \frac{1 - r^N}{1 - r} \tag{179}$$

2. Reversibility/reciprocity of the DFT Equations

We defined the DFT using W_N in Equations 174 and 175. In this section we use these equations to prove, mathematically, the reversibility of the DFT. That is, if we obtain the DFT of a sequence using Equation 144, we uniquely obtain the same sequence back through Equation 145.

We start with $x_n = \frac{1}{N}\sum_{k=0}^{N-1} C_k W_N^{-nk}$ and substitute in $C_k = \sum_{n=0}^{N-1} x_n W_N^{nk}$ into it. We will then try to show that the right side of this equation becomes x_n. Note that n performs different roles in $x_n = \frac{1}{N}\sum_{k=0}^{N-1} C_k W_N^{-nk}$ and $C_k = \sum_{n=0}^{N-1} x_n W_N^{nk}$. It plays the role of a 'frequency' in $x_n = \frac{1}{N}\sum_{k=0}^{N-1} C_k W_N^{-nk}$, but as a dummy variable in $C_k = \sum_{n=0}^{N-1} x_n W_N^{nk}$. Accordingly, before substituting

$C_k = \sum_{n=0}^{N-1} x_n W_N^{nk}$ we change n, the dummy variable, to j such that: $C_k = \sum_{j=0}^{N-1} x_j W_N^{jk}$, which gives:

$$x_n = \frac{1}{N}\sum_{k=0}^{N-1} C_k W_N^{-nk} = \frac{1}{N}\sum_{k=0}^{N-1}\left[\sum_{j=0}^{N-1} x_j W_N^{jk}\right] W_N^{-nk} \tag{180}$$

As is typical in these types of derivations (also with integrals – see above), we switch the order of these summations to obtain:

$$\frac{1}{N}\sum_{k=0}^{N-1} C_k W_N^{-nk} = \frac{1}{N}\sum_{j=0}^{N-1} x_j \sum_{k=0}^{N-1} W_N^{jk} W_N^{-nk} = \frac{1}{N}\sum_{j=0}^{N-1} x_j \sum_{k=0}^{N-1} W_N^{(j-n)k} \tag{181}$$

We now used the first summation to write out our equation as follows:

$$\begin{aligned} &\frac{1}{N}\sum_{k=0}^{N-1} C_k W_N^{-nk} \\ &\qquad = \frac{1}{N}\sum_{j=0}^{N-1} x_j \sum_{k=0}^{N-1} W_N^{(j-n)k} \\ &\qquad = \frac{1}{N}(x_0 \sum_{k=0}^{N-1} W_N^{(0-n)k} + x_1 \sum_{k=0}^{N-1} W_N^{(1-n)k} + \cdots \\ &\qquad + x_n \sum_{k=0}^{N-1} W_N^{(n-n)k} + \cdots + x_{N-1} \sum_{k=0}^{N-1} W_N^{(N-1-n)k} + \cdots) \end{aligned} \tag{182}$$

Now, there are two possibilities for $j-n$ in Equation 181. The first is that $j \neq n$. In this case, we use the sum of a finite geometric series that we just derived, which gives us:

$$\sum_{k=0}^{N-1} W_N^{(j-n)k} = 1 + \left(W_N^{(j-n)}\right)^1 + \left(W_N^{(j-n)}\right)^2 + \cdots + \left(W_N^{(j-n)}\right)^{N-1}$$ (183)

$$= \frac{1-\left(W_N^{(j-n)}\right)^N}{1-W_N^{(j-n)}}$$

However, $W_N = e^{-i2\pi/N}$ so $\left(W_N^{(j-n)}\right)^N = \left(e^{-i2\pi(j-n)/N}\right)^N = e^{-i2\pi(j-n)} = 1$. Thus, $\sum_{k=0}^{N-1} W_N^{(j-n)k} = \frac{1-\left(W_N^{(j-n)}\right)^N}{1-W_N^{(j-n)}} = \frac{1-1}{1-W_N^{(j-n)}} = 0$. Thus, every term in Equation 181 for which $j \neq n$ disappears, leaving us:

$$\frac{1}{N}\sum_{k=0}^{N-1} C_k W_N^{-nk} = \frac{1}{N}\sum_{j=0}^{N-1} x_j \sum_{k=0}^{N-1} W_N^{(j-n)k} = \frac{1}{N}\left(x_n \sum_{k=0}^{N-1} W_N^{(n-n)k}\right)$$ (184)

$$= \frac{1}{N}\left(x_n \sum_{k=0}^{N-1} 1\right) = \frac{1}{N} x_n N = x_n$$

which completes our proof.

J. *Inverse Property of the DFT: Taking the DFTs of Broader and Narrower Gaussians*

In this section, we create broader and narrower Gaussians and show that, as expected, the DFT of the broader Gaussian is narrower. The commands listed below for making these Gaussians and taking their DFTs are in MATLAB. Please note that variables do not need to be predefined in MATLAB. One defines a variable by writing it at the command line (>>) and associating it with a mathematical operation.

A broader Gaussian (Figure 27) was created in MATLAB using the following code:

```
>> xvals = 1:64                                          (185)
>> yvals = exp(-0.01.*(xvals-30).^2)
>> plot(xvals, yvals), shg
```

That is, `1:64` creates a vector consisting of the numbers [1 2 3 4 … 64], `yvals` creates a shifted Gaussian with a center at 30 and defines its width, and `shg` stands for 'show graph'. Please note that while the MATLAB commands shown in this text do recreate the figures in the text, extra formatting, which is not listed here, has been added to these figures to make the lines in them heavier, add color to them, etc.

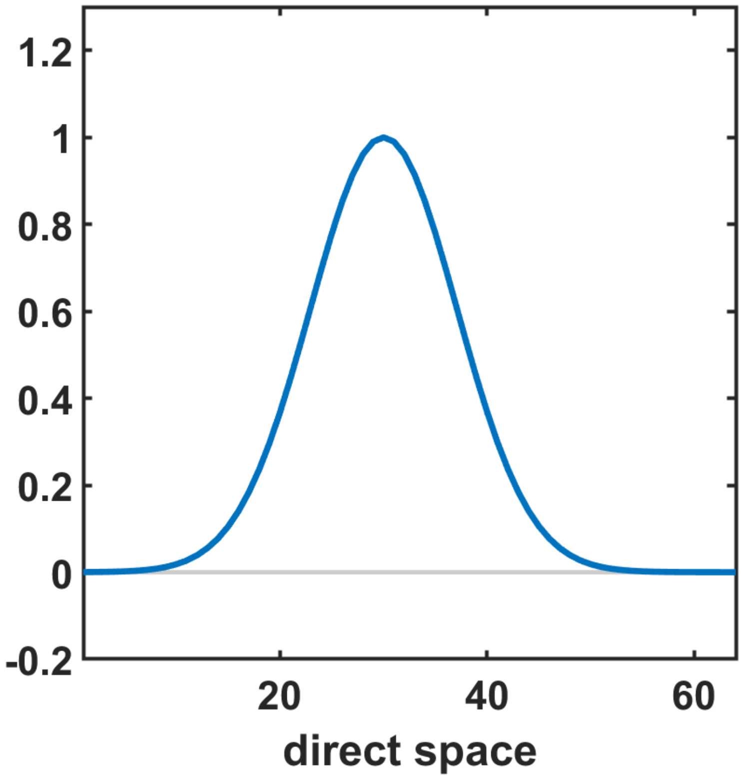

Figure 27. A broader Gaussian based on 64 data points. See Equation 185 for the MATLAB code used to make it.

We now take the DFT of `yvals` in Equation 185 and plot the real and imaginary parts of it. The MATLAB command for taking the DFT is `fft`.

```
>> fft_yvals = fft(yvals)
```
(186)

Next, we take the real part of `fft_yvals` from Equation 186 and plot it (see Figure 28) using the commands:

```
>> fft_yvals_real = real(fft_yvals)
>> plot(xvals, fft_yvals_real), shg
```
(187)

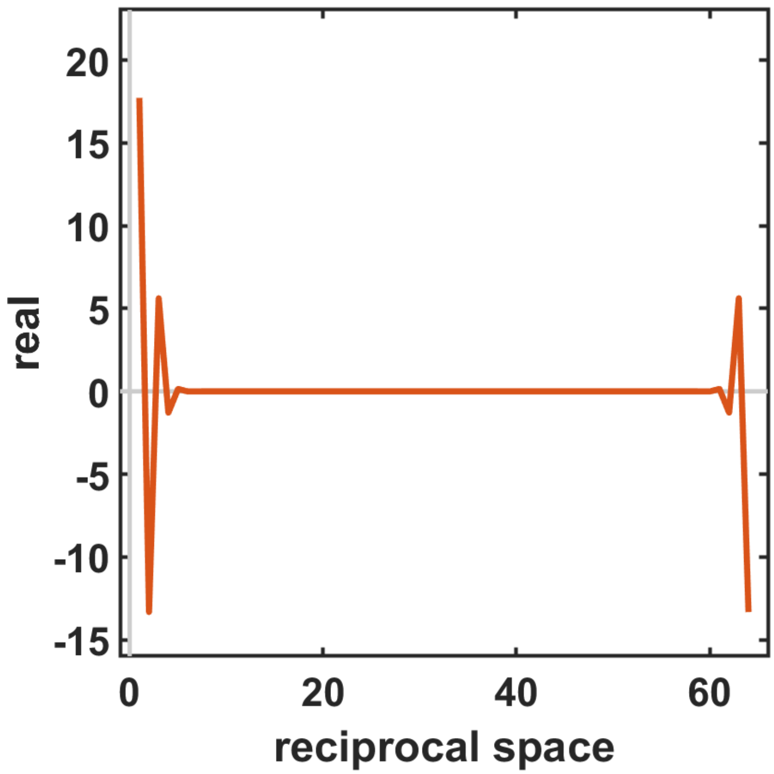

Figure 28. The real part of the DFT of the Gaussian shown in Figure 27 generated with the commands in Equation 187.

And we then take the imaginary part of `fft_yvals` and plot it (Figure 29) using the following commands:

```
>> fft_yvals_imag = imag(fft_yvals)
>> plot(xvals, fft_yvals_imag), shg
```
(188)

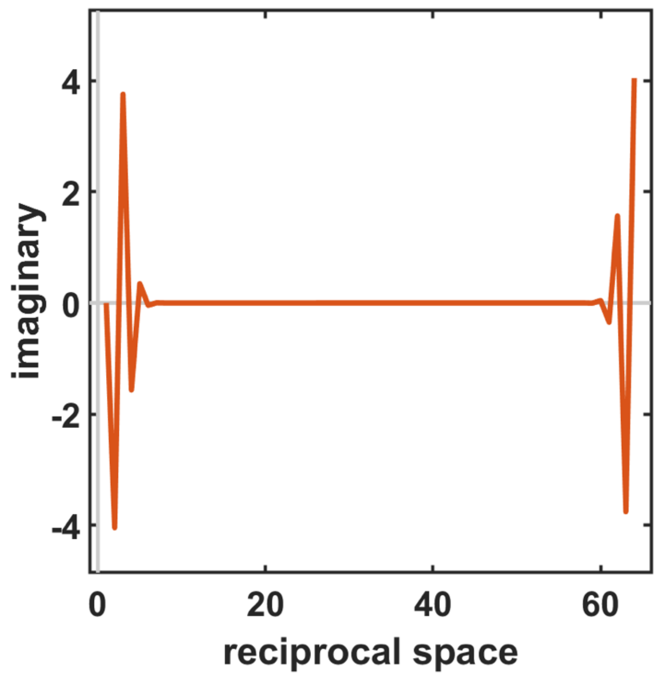

Figure 29. The imaginary part of the DFT of the Gaussian shown in Figure 27 generated with the commands in Equation 188.

While Figure 28 and Figure 29 are legitimate ways of viewing a DFT, it is more common to plot the modulus (magnitude) of the values of a DFT, which we obtain and plot in Figure 30 as follows:

```
>> fft_yvals_mod = sqrt(fft_yvals_real.^2 + fft_yvals_imag.^2)
>> plot(xvals, fft_yvals_mod), shg
```
(189)

The phase, which is the arctan of the imaginary part of the DFT divided by the real part, may or may not be shown. That is, when data are denoised, it is sometimes ignored. When the phase is not shown, the modulus only reveals to us that particular frequencies, including spatial frequencies, are used to make up or not make up a function in direct space, but it does not tell us whether these frequencies correspond to sines or cosines in the underlying Fourier analysis. Please note that while, in Equation 180, we explicitly showed how to obtain the modulus of a complex number, MATLAB has a command to do this directly, which is `abs`.

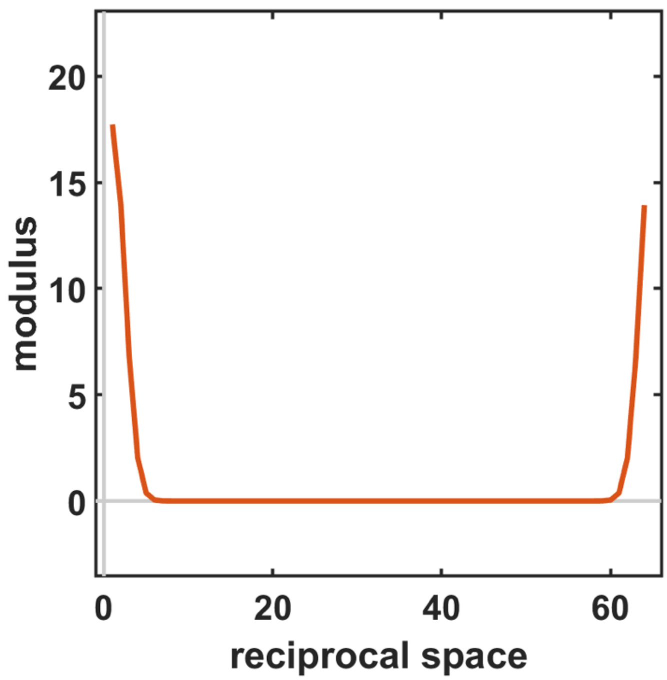

Figure 30. The modulus of the DFT of the broader Gaussian shown in Figure 27 generated with the commands in Equation 189.

We now create a narrower Gaussian than the one in Example 1 (Figure 27) and examine its DFT. Figure 31 shows this narrower Gaussian, and Figure 32 shows the modulus of its DFT, which were made as follows:

```
>> yvals_nar = exp(-0.1.*(xvals-30).^2)
>> plot(xvals, yvals_nar), shg
```
(190)

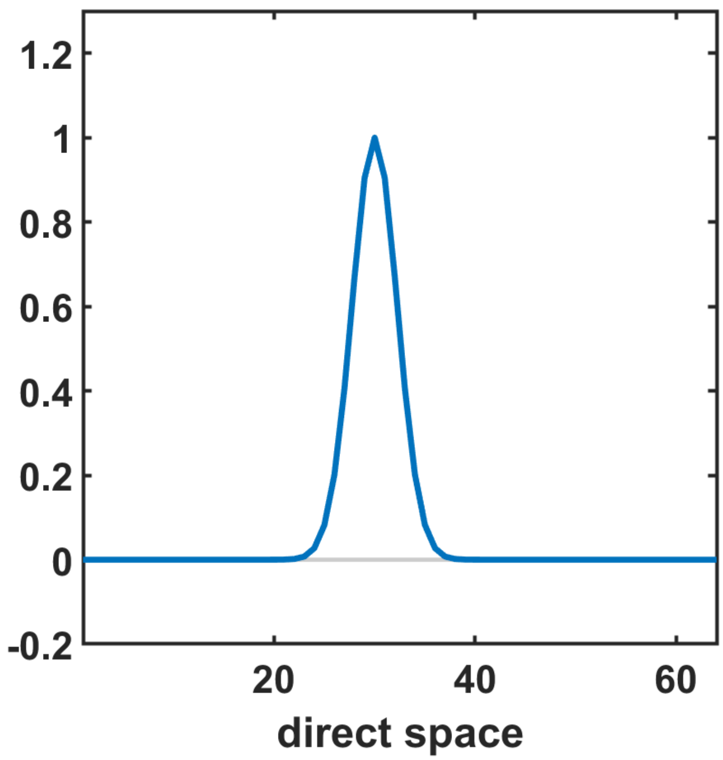

Figure 31. A narrower Gaussian based on 64 data points. See Equation 190 for the MATLAB code used to make it.

We now take the DFT of this narrower Gaussian and plot its modulus (Figure 32), as follows:

```
>> fft_yvals_nar = fft(yvals_nar)
>> plot(xvals, abs(fft_yvals_nar)), shg
```
(191)

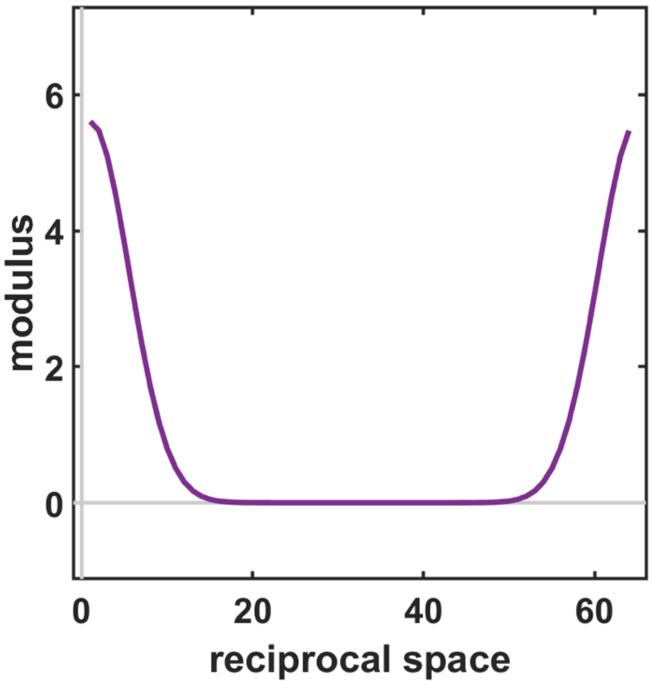

Figure 32. The modulus of the DFT of the Gaussian shown in Figure 31 generated with the commands in Equation 191.

Figure 33 shows a plot of the moduli of the DFTs of the broader (Figure 27) and narrower (Figure 31) Gaussians just created and discussed. As expected, the DFT of the narrower Gaussian is broader, and vice versa. Fewer meaningful Fourier coefficients are required to recreate the broader Gaussian.

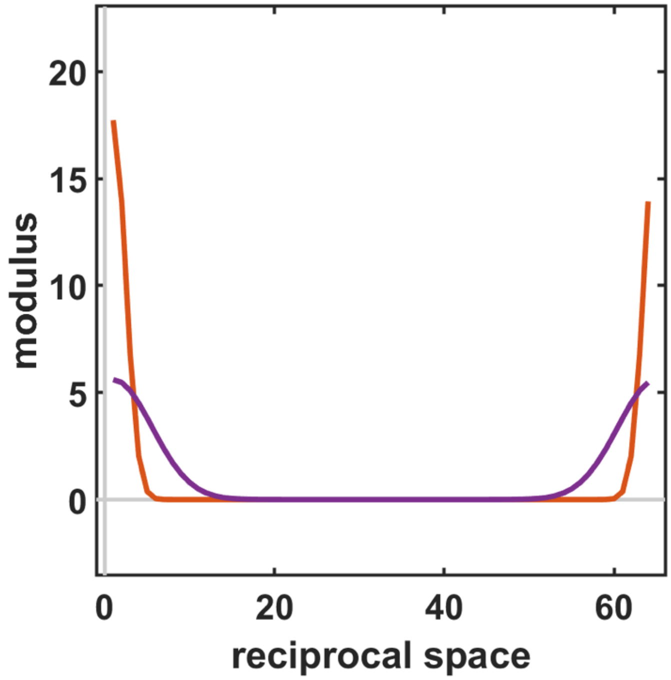

Figure 33. The moduli of the DFTs of the broader (Figure 27) and narrower (Figure 30) Gaussians just created and discussed, which are orange and purple, respectively. That is, the DFT of the broader Gaussian is narrower.

K. *Noise Removal from a Noisy Gaussian*

This section is directly relevant to the problem of removing noise from data. In it, we take the simplistic approach of zeroing out high-frequency Fourier coefficients that contain noise, which produces a denoised signal in direct space.

We first create of a noisy version of the Gaussian in Figure 27 and then calculate its DFT. That is, we add normally distributed, random numbers to the peak contained in `yvals` (the peak in Figure 27) as follows:

```
>> yvals_noise = yvals + 0.05*randn(1,64)
>> plot(xvals, yvals_noise), shg
```
(192)

By adding noise to our original, smooth Gaussian we have added high frequency information to it.

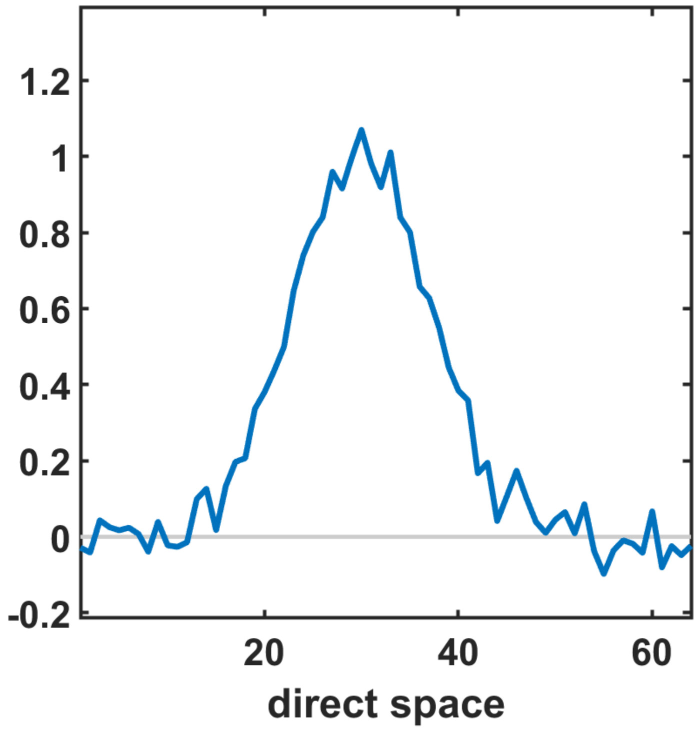

Figure 34. The Gaussian peak in Figure 27 with random noise added to it. See Equation 192.

We now take the modulus of the DFT of the data in Figure 34 and plot it in Figure 35, as follows:

```
>> plot(xvals, abs(fft(yvals_noise))), shg
```
(193)

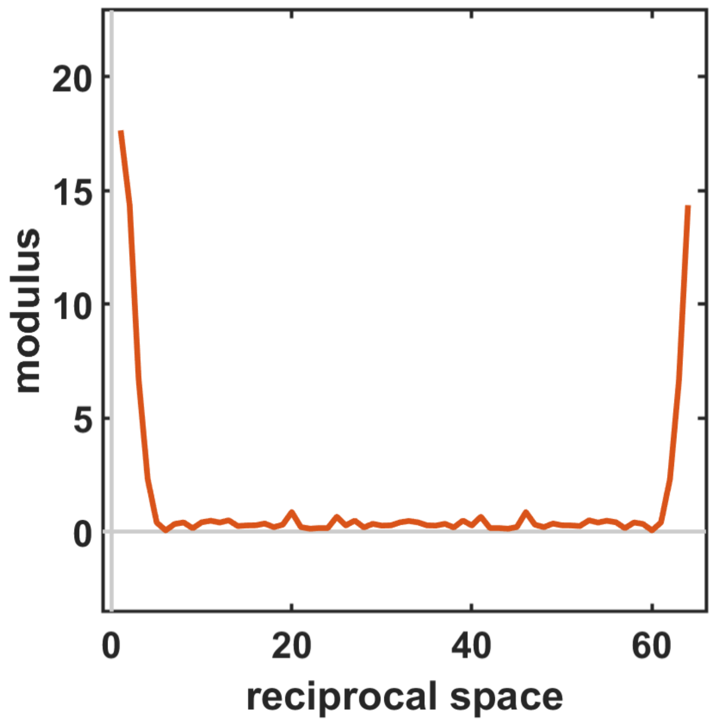

Figure 35. Modulus of the DFT of the noisy Gaussian in Figure 34.

As expected, higher frequency, non-zero Fourier coefficients become obvious.

In Figure 36, we overlay the moduli of the Fourier coefficients of the noisy (Figure 35) and noise-free (Figure 30) broader Gaussians using the following code:

```
>> plot(xvals, abs(fft(yvals_noise))), hold on
>> plot(xvals, abs(fft(yvals))), shg
```

(194)

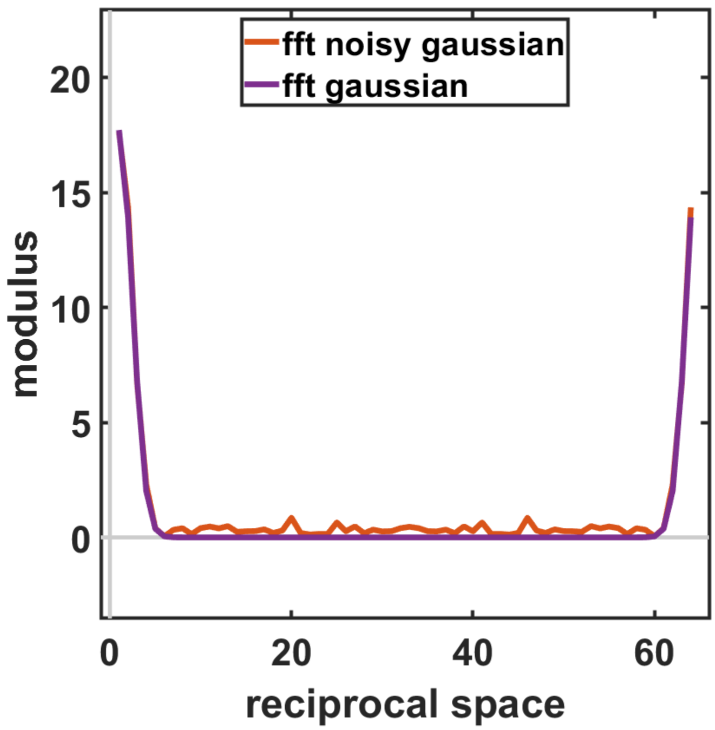

Figure 36. Overlay of the moduli of the DFTs of the Gaussians in Figure 30 and Figure 35.

Just to confirm that there is noise in both the real and imaginary parts of the DFT of our noisy Gaussian, we plot the real and imaginary parts of them with the real and imaginary parts of the DFT of the noise-free Gaussian in Figure 37 and Figure 38, respectively, using the following segments of code:

```
>> plot(xvals, real(fft(yvals_noise))), hold on
>> plot(xvals, real(fft(yvals))), shg
```
(195)

and

```
>> plot(xvals, imag(fft(yvals_noise))), hold on
>> plot(xvals, imag(fft(yvals))), shg
```
(196)

where these figures do indeed show noisy, higher-order Fourier coefficients where they were essentially zero before.

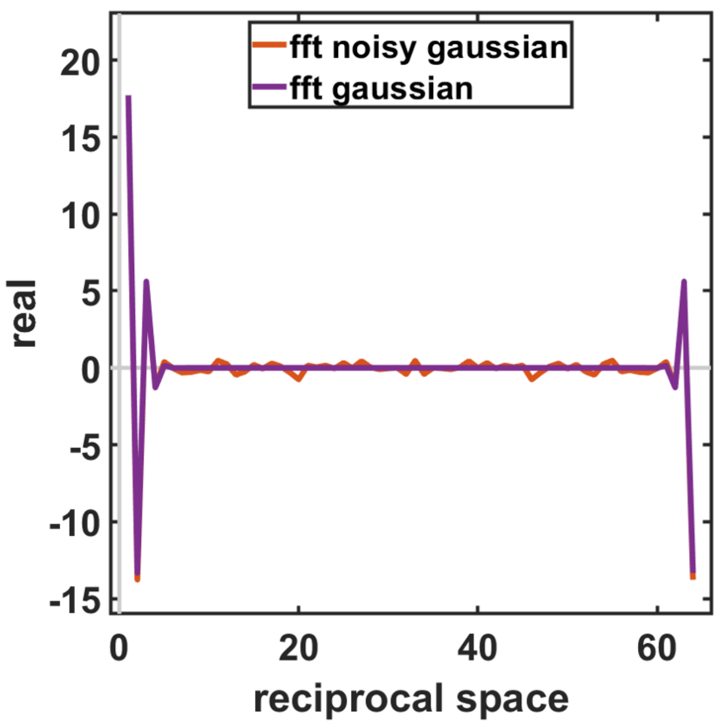

Figure 37. Real parts of the DFTs of the broader, noise-free and noisy Gaussians in Figure 27 and Figure 34, respectively.

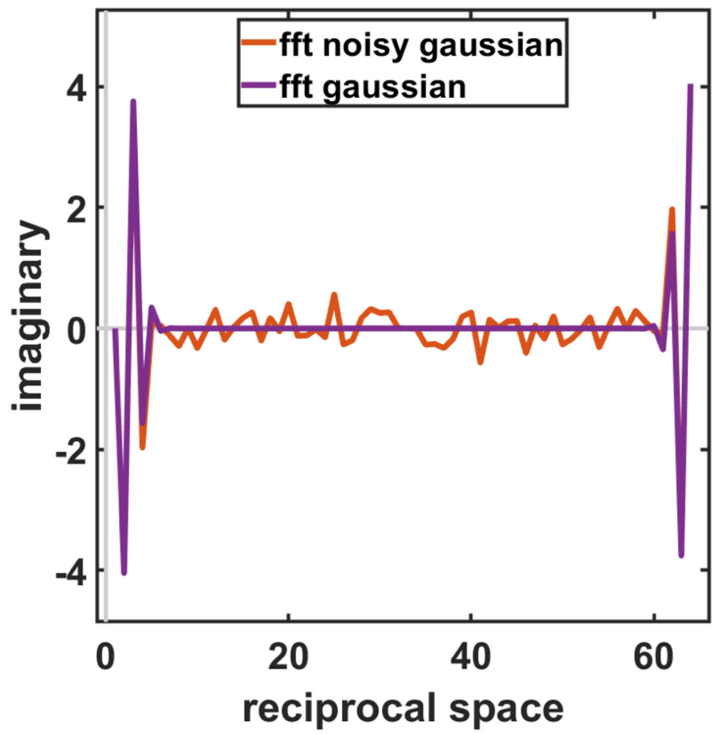

Figure 38. Imaginary parts of the DFTs of the broader, noise-free and noisy Gaussians in Figure 27 and Figure 34, respectively.

In a simplistic way, we now zero out the Fourier coefficients from the noisy Gaussian that are primarily a result of noise, revealing a basic process/strategy for removing the noise from a noisy spectrum in reciprocal space. As shown in Figure 36 - Figure 38, in the low-frequency region of the DFT, the Fourier coefficients of the noisy and noise-free Gaussians are very similar. However, as already noted, the noisy Gaussian shows larger Fourier coefficients in the middle regions of these DFTs, which are due to noise. Accordingly, we zero out the Fourier coefficients from ca. positions 6 – 60 in the DFT of the noisy Gaussian and plot them in Figure 39 with the following code:

```
>> fft_yvals_noise = fft(yvals_noise)
>> fft_yvals_noise_filtered = fft_yvals_noise
>> fft_yvals_noise_filtered([6:60]) = 0
>> plot(xvals, abs(fft_yvals_noise_filtered)), hold on
>> plot(xvals, abs(fft_yvals_noise)), shg
```
(197)

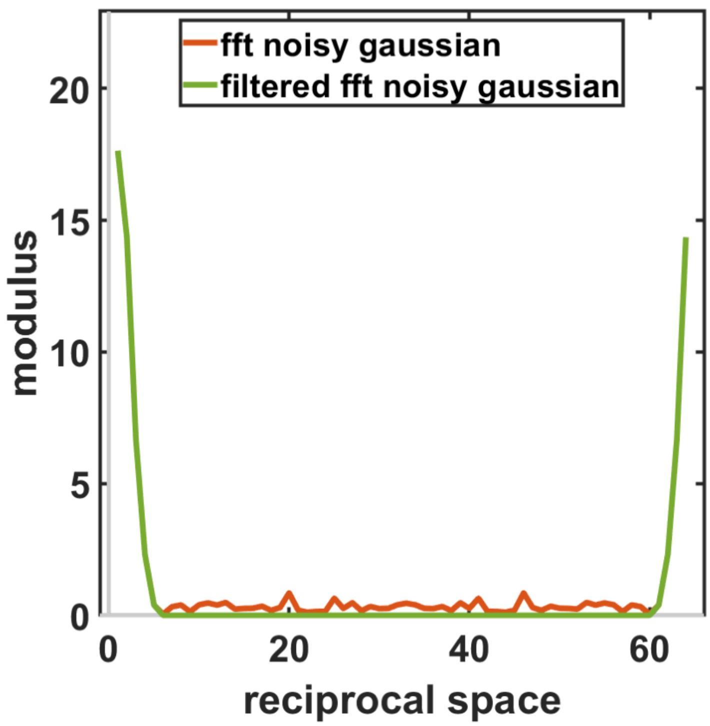

Figure 39. The modulus of the DFT of the noisy Gaussian plotted in Figure 34 and the same Fourier coefficients after those between positions 6 and 60 were zeroed out.

We now take the inverse Fourier transform of our filtered DFT and plot it on top of our original Gaussian and noisy Gaussian in Figure 40, as follows:

```
>> ifft_fft_yvals_noise_filtered =
ifft(fft_yvals_noise_filtered)
>> plot(xvals, ifft_fft_yvals_noise_filtered), hold on
>> plot(xvals, yvals_noise)
>> plot(xvals, yvals), shg
```
(198)

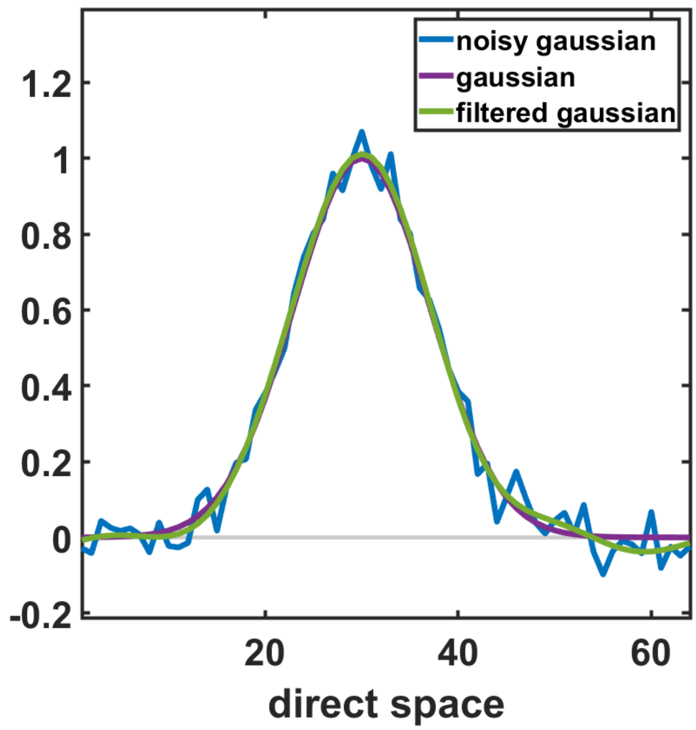

Figure 40. Overlay of the noise-free Gaussian in Figure 27, the noisy Gaussian in Figure 34, and the signal produced by denoising the noisy Gaussian in Figure 34.

It is remarkable how close the smoothed Gaussian is to the original, noise-free Gaussian. Note that variations in the denoised Gaussian that are about the same size, or smaller, than the noise on the noisy Gaussian should not be considered to be real.

L. *Theorems of the DFT*

In general, the DFT has theorems that are analogous to those of the Fourier transform, and they are important for similar reasons. They often allow results to be obtained more quickly than would otherwise be possible. For example, in some cases, a proved theorem will be helpful in proving another theorem.

1. Addition, Sum, or Linearity Theorem

Suppose $\{x_i\}_{i=1}^{n} = x_i$ and $\{y_i\}_{i=1}^{n} = y_i$ are sequences of the same length (n), and their DFTs are $\{C_j\}_{j=1}^{n} = C_j$ and $\{D_j\}_{j=1}^{n} = D_j$, respectively. Then:

$$DFT[x_i + y_i] = C_j + D_j \tag{199}$$

Furthermore, if a and b are constants:

$$DFT[ax_i + by_i] = aC_j + bD_j \tag{200}$$

We can prove Equation 200 by writing:

$$\begin{aligned} &DFT[ax_i + by_i] \\ &= \sum_{n=0}^{N-1} (ax_i + by_i) e^{-i2\pi k(n/N)} \\ &= \sum_{n=0}^{N-1} \left(ax_i e^{-i2\pi k(n/N)} + by_i e^{-i2\pi k(n/N)}\right) \\ &= a\sum_{n=0}^{N-1} x_i e^{-i2\pi k(n/N)} + b\sum_{n=0}^{N-1} y_i e^{-i2\pi k(n/N)} = aC_j + bD_j \end{aligned} \tag{201}$$

where the first result (in Equation 199) is proved by taking $a = b = 1$ in Equation 201.

2. First shifting theorem

Weaver refers to this theorem as the 'first shifting theorem'.[9] To prove it, assume that x_i and its DFT, C_k, are sequences of length N. Suppose we shift our sequence by a certain number of positions, s, to create a new sequence x_{i-s}. What is the DFT of x_{i-s}? Note that, to create our new sequence, we will invoke the periodic nature of sequences in the DFT. For example, suppose $N = 8$, $\{x_i\}_{i=1}^{7} = x_i = \{1, 2, 0, 4, 7, -8, -3, -2\}$, and $s = 2$. The new sequence, x_{i-2}, is $\{-3, -2, 1, 2, 0, 4, 7, -8\}$. We will use $W_N = e^{-i2\pi/N}$ and $x_n = \frac{1}{N}\sum_{k=0}^{N-1} C_k W_N^{-nk}$ (Equation 175) in this derivation.

$$x_{n-s} = \sum_{k=0}^{N-1} C_k W_N^{-(n-s)k} = \sum_{k=0}^{N-1} C_k W_N^{-nk} W_N^{sk} = \sum_{k=0}^{N-1} \left(C_k W_N^{sk}\right) W_N^{-nk} \tag{202}$$

That is, $x_{n-s} = DFT^{-1}\left(C_k W_N^{sk}\right)$, which implies that $DFT(x_{n-s}) = C_k W_N^{sk}$. In other words, when a sequence is shifted in direct space, its DFT is multiplied by a sinusoidal term, W_N^{sk}, where the size of the shift, s, dictates the frequency of the sinusoidal term.

3. *Second shifting theorem*

Weaver refers to this theorem as the 'second shifting theorem'.[9] We will not use the weighting kernel in its derivation. Consider a sequence, x_j, of length, N, with DFT C_k: $C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)}$. What is the DFT of $x_j e^{-i2\pi js/N}$, where s is a constant? We proceed as follows:

$$DFT\left(x_j e^{-i2\pi js/N}\right) = \sum_{n=0}^{N-1} x_n e^{-i2\pi ns/N} e^{-i2\pi k(n/N)} \tag{203}$$

$$= \sum_{n=0}^{N-1} x_i e^{-i2\pi(s+k)n/N} = C_{s+k}$$

In other words, multiplying a sequence by a complex exponential, $e^{-i2\pi js/N}$, shifts the Fourier coefficients of the sequence.

4. The modulation theorem for DFTs

If a sequence, x_j, of length, N, has a DFT of C_k, what is the DFT of $x_j \cos(\frac{2\pi js}{N})$? To show this theorem, we use the second shifting theorem, which states: $DFT\left(x_j e^{-i2\pi js/N}\right) = C_{s+k}$. It follows that: $DFT\left(x_j e^{i2\pi js/N}\right) = C_{-s+k}$. Thus, we write out:

$$x_j e^{-i2\pi js/N} = x_j\left(cos(2\pi js/N) - isin(2\pi js/N)\right) \tag{204}$$

$$x_j e^{i2\pi js/N} = x_j\left(cos(2\pi js/N) + isin(2\pi js/N)\right) \tag{205}$$

Adding Equations 204 and 205 gives:

$$x_j e^{-i2\pi js/N} + x_j e^{i2\pi js/N} = 2x_j cos(2\pi js/N) \tag{206}$$

Accordingly:

$$DFT\left(x_j e^{-i2\pi js/N}\right) + DFT\left(x_j e^{i2\pi js/N}\right) = DFT\left(x_j e^{-i2\pi js/N} + x_j e^{i2\pi js/N}\right) \tag{207}$$

$$= DFT\left(2x_j cos(2\pi js/N)\right) = C_{s+k} + C_{-s+k}$$

And, thus: $x_j cos(2\pi js/N) \leftrightarrow \frac{1}{2}(C_{s+k} + C_{-s+k})$.

If instead of adding Equations 204 and 205 we subtract them, we obtain:

$$x_j e^{-i2\pi js/N} - x_j e^{i2\pi js/N} = -2ix_j sin(2\pi js/N) \tag{208}$$

Similar logic reveals that: $x_j sin(2\pi js/N) \leftrightarrow \frac{i}{2}(C_{s+k} - C_{-s+k})$.

5. *The DFT of the DFT*

If a sequence, x_j, of length, N, has a DFT of C_k, what is $DFT\left(DFT(x_j)\right)$?

We proceed as follows:

$$DFT\left(DFT(x_j)\right) = DFT(C_k) = \sum_{k=0}^{N-1} C_k e^{-i2\pi jk/N} = N\left(\frac{1}{N}\sum_{k=0}^{N-1} C_k e^{i2\pi(-j)k/N}\right) \tag{209}$$

$$= Nx_{-j}$$

This result is analogous to the result we obtained for the Fourier transform of the Fourier transform in Equation 118.

Conclusions

In conclusion, we have described the Fourier transform and discrete Fourier transform in general, and also several of the detailed mathematical aspects associated with them. The discrete Fourier transform provides an effective and powerful way for removing noise from data.

Statement of Attribution

This document was written by Linford. Gerashchenko made the very nice figures and did the referencing. Gerashchenko also checked the document with ChatGPT, which found a few errors in it, which were corrected, and made other suggestions, some of which were taken.

Acknowledgments

We wish to thank David E. Aspnes for his useful comments on this document.

Data Availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Author Declarations

Conflict of interest. The main author on this article has recently started a software company (Fourier-AI Innovations, LLC) that is based on the Fourier denoising of data.

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