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A Tutorial on the Fourier Transform and Discrete Fourier Transform, with Comments on the Hilbert Transform, in the Context of Denoising Spectra

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ABSTRACT

In another article in this special collection,¹ 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, e.g., in two dimensions, in the context of denoising spectra. It also discusses the Hilbert transform, which is generally calculated in reciprocal space via Fourier analysis. That is, after some introductory words, which motivate the topic, this article 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, the discrete Fourier transform, and the Hilbert transform. Even a partial understanding of this material should help those who wish to use Fourier theory use it more successfully. The Fourier transform and discrete Fourier transform are powerful tools for data analysis.

I. MOTIVATION

X-ray photoelectron spectrometer (XPS) manufacturers are creating 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 during 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, where 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 also discusses the Hilbert transform, which is often applied in reciprocal space via Fourier analysis. 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.

II. 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 'Monty 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 denied. 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.

III. 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. As noted previously,¹ and expounded on a little more here, in many types of spectroscopy, including XPS, signal is a result of point-to-point correlations, while noise is a result of point-to-point fluctuations, i.e., for XPS this is because of the Poisson counting/statistics present in XPS data collection. 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 (Fourier) 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-Golay² 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 result from the polynomial (at that central point). 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 a small number of adjacent data points in a spectrum 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, in general, 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 also discuss the Hilbert transform. 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, and especially to those without strong math backgrounds. 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 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, 6-24}

In addition, this work follows previous analyses of XPS data, including efforts to denoise it with wavelets,²⁵⁻²⁸ and also analyses of whole spectra as vectors (in hyperspaces) using techniques that include principal component analysis (PCA),²⁹⁻³¹ multivariate curve resolution (MCR),³² and cluster analysis.³³

IV. 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 later 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 via Fourier analysis.

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 were added together previously to make it. Both the frequencies and amplitudes of these underlying waves matter.

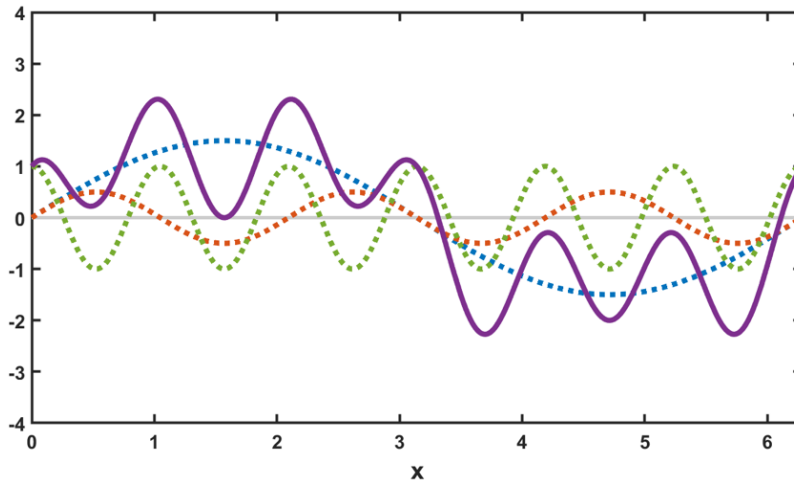


Figure 1. A function (solid purple line) created by summing a 'blue' sinusoid: $1.5 \sin(x)$, an 'orange' sinusoid: $0.5 \sin(3x)$, and a 'green' sinusoid: $\cos(6x)$.

The Fourier transform is commonly defined as follows:

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

and the inverse Fourier transform as:

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

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: $\mathcal{F}\{f(x)\}(s) = \mathcal{F}\{f(x)\} = \mathcal{F}f(x) = \mathcal{F}f = F(s) = F$, 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, $\mathcal{F}\mathcal{F}f = f$ when f is an even function, which is an important special case.

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

$$e^{ix} = \cos(x) + i\sin(x) \quad (3)$$

Thus, for Equations 1 and 2 we can write:

$$e^{-i2\pi sx} = \cos(2\pi sx) - i\sin(2\pi sx) \quad (4)$$

and

$$e^{i2\pi sx} = \cos(2\pi sx) + i\sin(2\pi sx) \quad (5)$$

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 (an 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 really exist. Rather, they often end up being a mathematical convenience in Fourier theory. At least theoretically, when we perform a Fourier transform, we need to do an integral for every possible value of s .

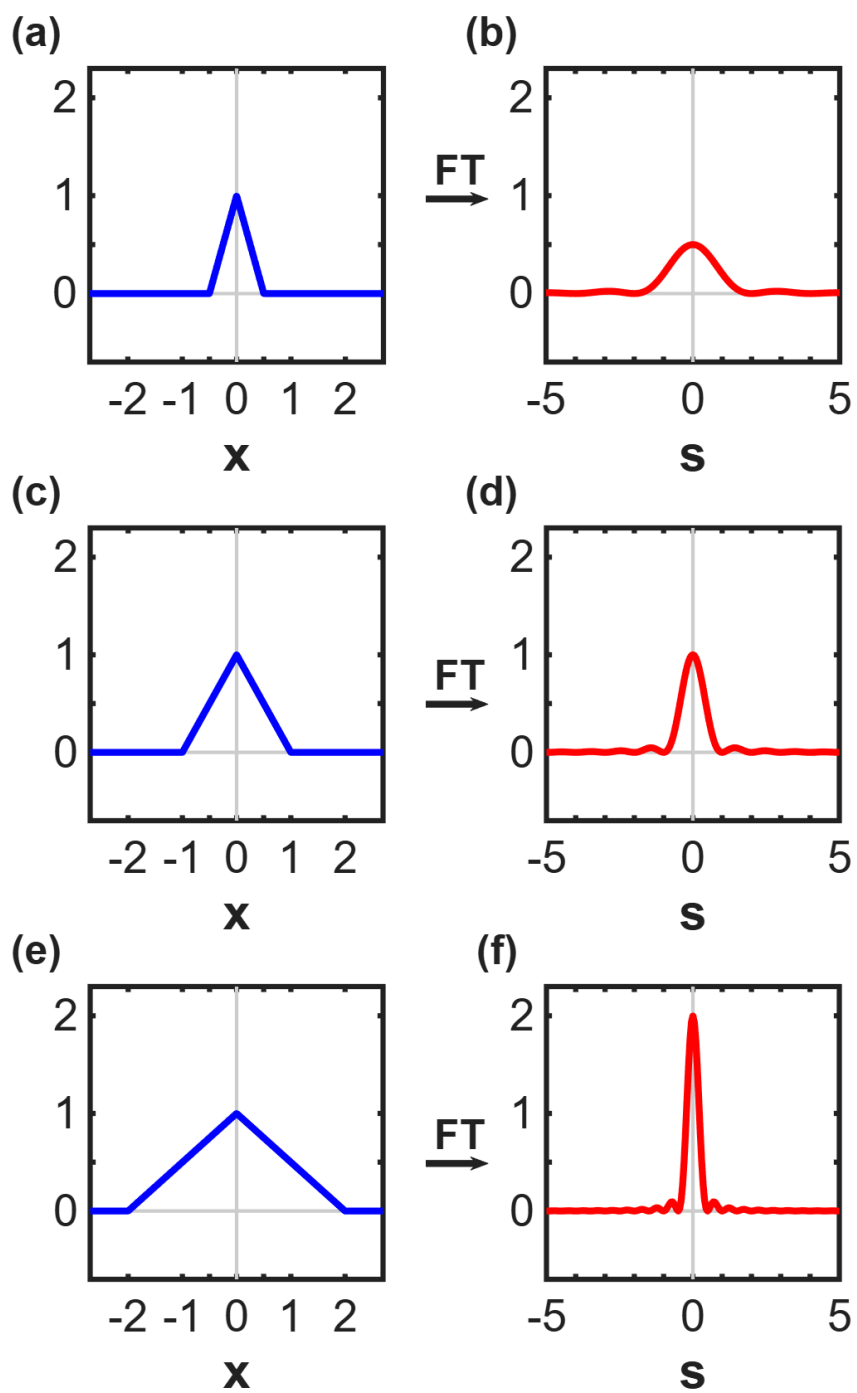


Figure 2. (a, c, and e) Three triangle functions with different widths and (b, d, and f) their respective Fourier transforms.

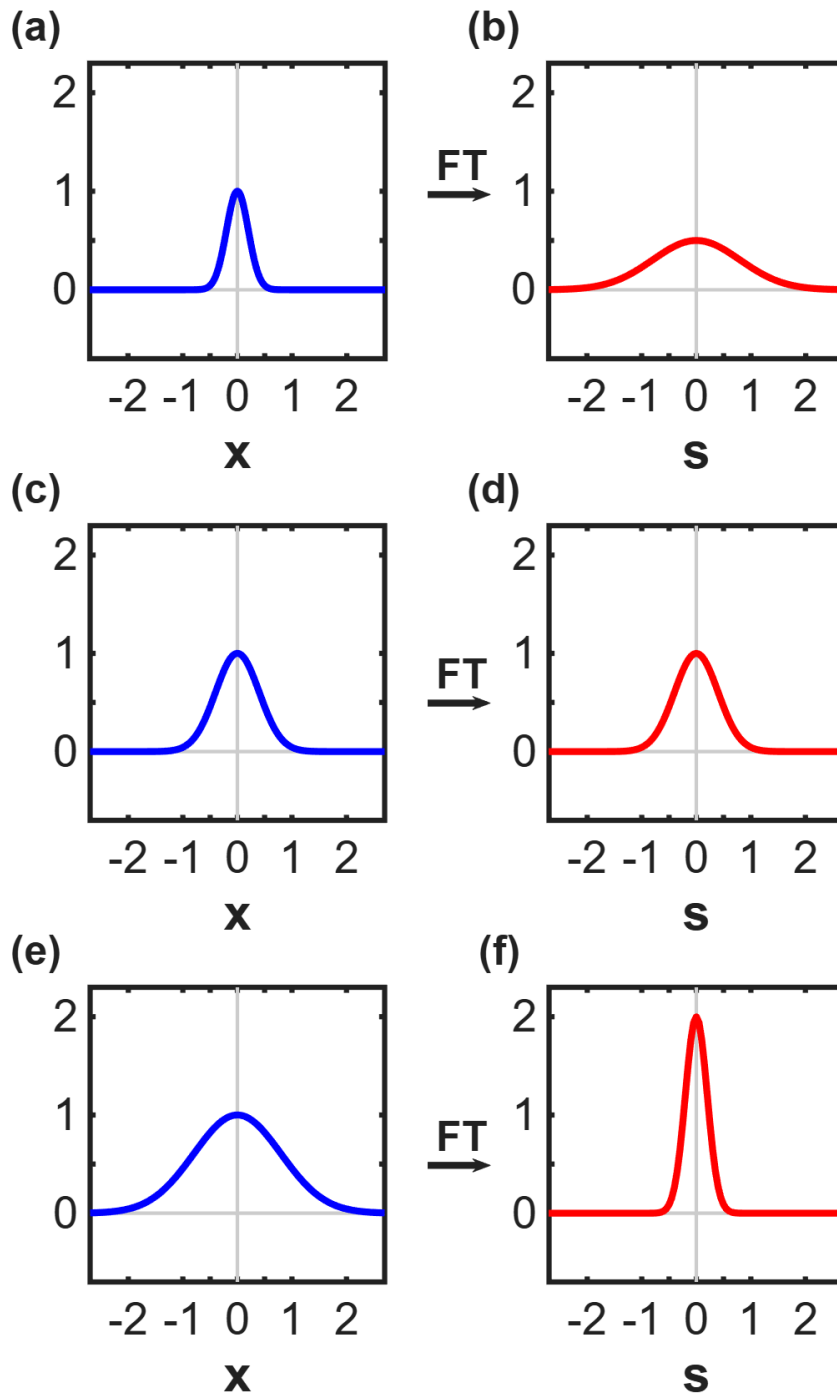


Figure 3. (a, c, and e) Three Gaussian functions with different widths and (b, d, and f) their respective Fourier transforms.

The Fourier transform has an important reciprocal property. Broader functions have narrower Fourier transforms, and narrower functions and/or functions with sharp features, have broader Fourier transforms. In other words, broader functions are made up of fewer frequency components, and it takes more frequency components to recreate narrow functions or sharp features. For example, Figure 2 shows three triangle functions that become broader. The Fourier transforms of these functions change oppositely to become narrower. 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, which remains unchanged. 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 light is passed across a slit. A convolution also

takes place when an X-ray beam is passed across a sharp interface between two different materials, which is done to determine its size.³⁴

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 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. Because the convolution of two functions in direct space produces another function in direct space, we need to back transform $F(s)G(s)$ to get $f(x) * g(x)$.

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 the 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. However, there are additional advantages to working in reciprocal space in spectral analysis that are at least as great as the advantage of greater computational speed. It is of considerable importance that the reciprocal space representation of a typical 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 noted previously,¹ this approach is inherently better than the traditional Savitzky-Golay² 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.

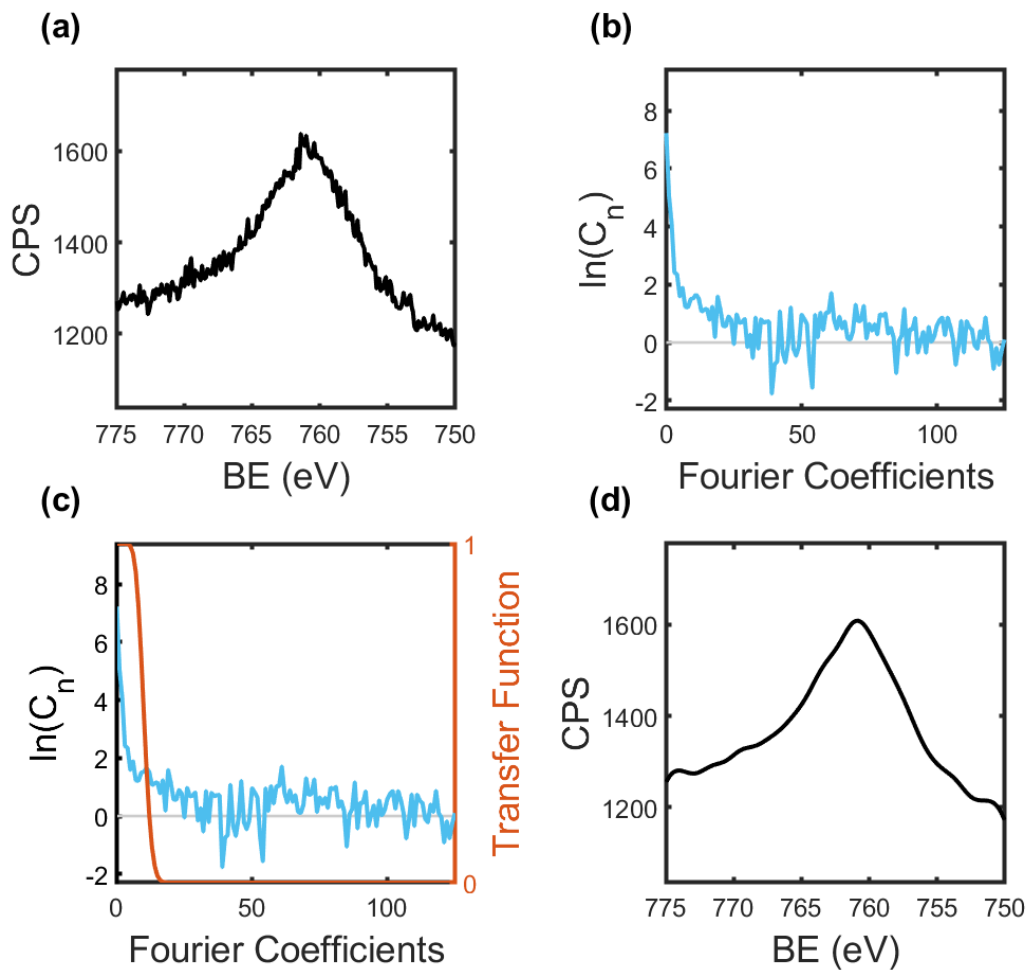


Figure 4. (a) An XPS narrow scan in direct space. (b) The DFT of the narrow scan in (a). (c) A Gauss-Hermite transfer function (orange) positioned on the DFT in (b). (d) The result of back transforming the product of the DFT and transfer function in (c).

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). The lower-index Fourier coefficients in Figure 4b describe the underlying signal in the spectrum, and the higher-index Fourier coefficients describe the noise in it. Note that Figure 4b and Figure 4c are plotted on log scales. Figure 4c shows the so-called Gauss-Hermite transfer function,³⁵⁻³⁷ 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 it is nearly zero for the 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. The smooth, curved shape of the Gauss-Hermite filter is also preferred over a transfer function with an abrupt cutoff in reciprocal space, i.e., a transfer function that multiplies the lower-index coefficients by unity and the higher-index coefficients by zero (above a threshold).¹ An abrupt cutoff can introduce artifacts into the original data, especially if features are very narrow. Fortunately, small deviations from what might be considered optimal positioning for the Gauss-Hermite 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. One should be skeptical of fluctuations in a denoised signal that are the same size or smaller than the noise in the original spectrum. We recommend that the original data always be shown with any denoised version of it.

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 provided below.

V. The Fourier Transform

A. Definitions of the Fourier transform

1. Definitions of the forward and inverse Fourier transforms

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

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

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 .”³⁸ 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:

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

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:

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

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:

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

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:

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

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 rather humorous. Different authors have different preferences, and a few authors can be rather insistent on the equations they prefer. Equations 6 and 9 were 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/simple, 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), and, e.g., $\cos(2\pi ft)$ and $\sin(2\pi ft)$ have undergone one cycle when $t = 1/f$, (v) are widely, but not exclusively, used, and (vi) are well accepted. Accordingly, Equations 6 and 9 will be used in this work.

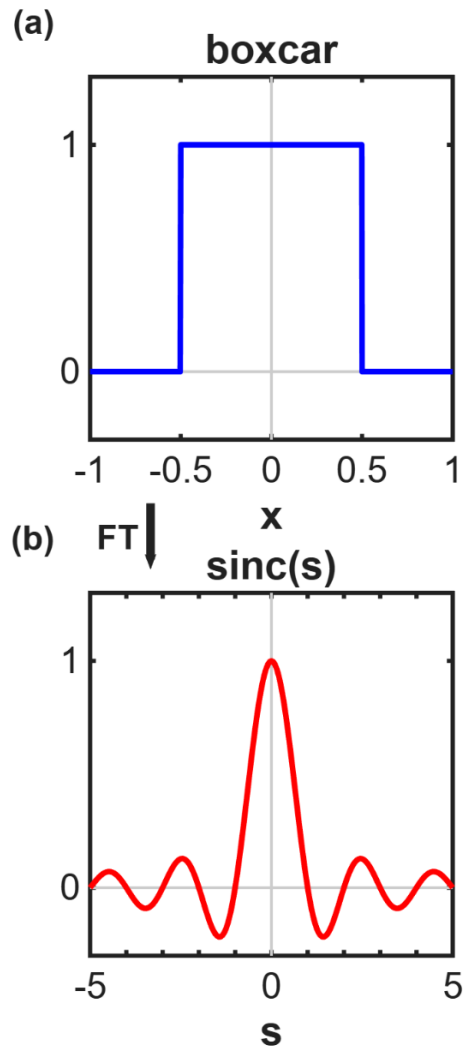


Figure 5. (a) The boxcar function, as defined in Equation 11, and its Fourier transform (b) the $\text{sinc}(s) = \frac{\sin(\pi s)}{\pi s}$ function.

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:

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

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:

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

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:

$$\begin{aligned}
F(s) &= \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx} dx = \int_{-\infty}^{\infty} \Pi(x)e^{-i2\pi sx} dx & (13) \\
&= \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{-i2\pi sx} dx = \frac{-1}{i2\pi s} e^{-i2\pi sx} \Big|_{-\frac{1}{2}}^{\frac{1}{2}} = \frac{i}{2\pi s} (e^{-i\pi s} - e^{i\pi s}) \\
&= \frac{i}{2\pi s} (\cos(\pi s) - i\sin(\pi s) - \cos(\pi s) - i\sin(\pi s)) = \frac{\sin(\pi s)}{\pi s} \\
&= \text{sinc}(s)
\end{aligned}$$

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 $\text{sinc}(s)$ 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 $\text{sinc}(s)$ are a Fourier transform pair, which we can represent as $\Pi(x) \leftrightarrow \text{sinc}(s)$. We will encounter other interesting Fourier transform pairs below.

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

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.

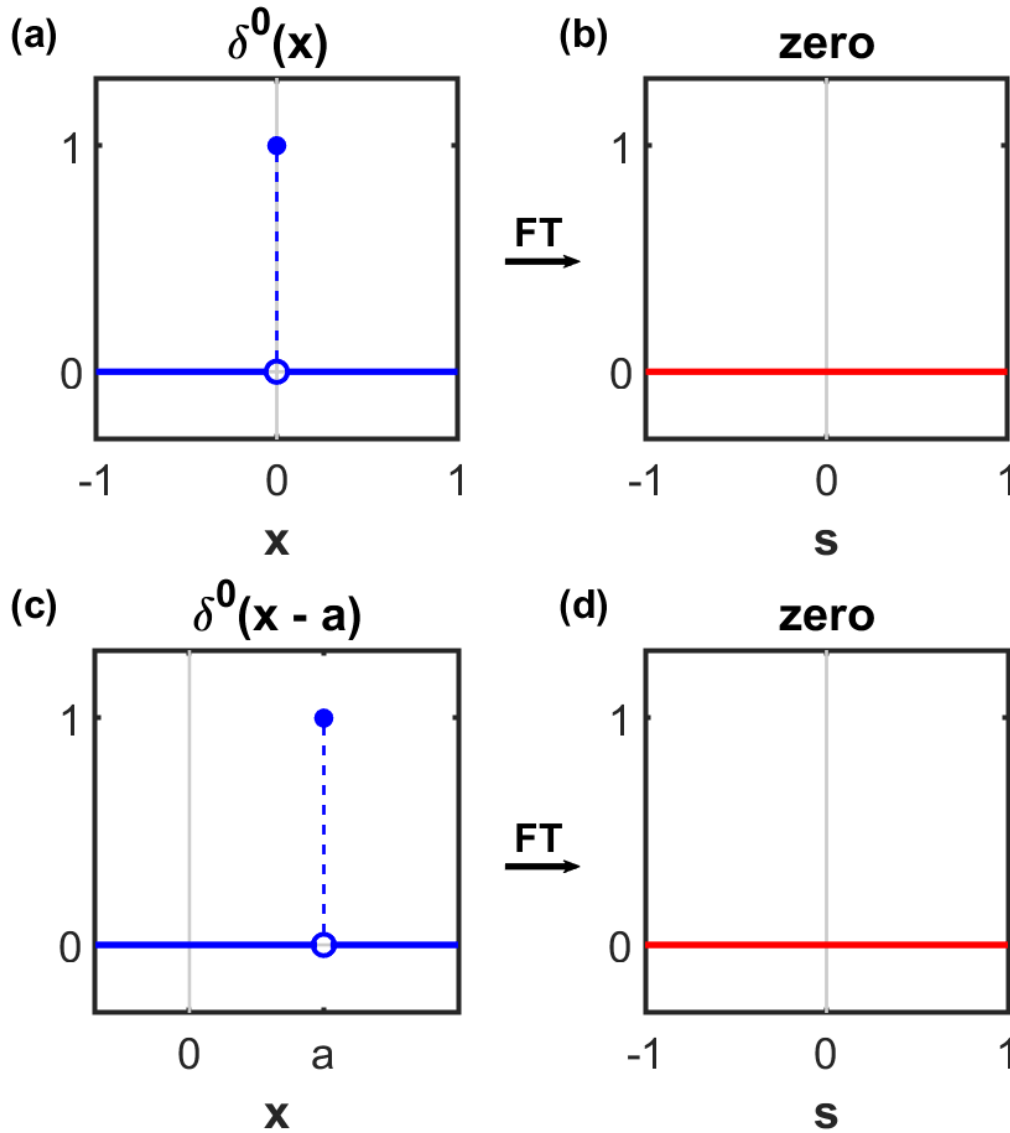


Figure 6. (a) Representation of the null function, $\delta^0(x)$, defined in Equation 15 and (b) its Fourier transform, which is zero. (c) Representation of the null function $\delta^0(x-a)$, as defined in the text, and (d) its Fourier transform, which is zero.

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:

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

For example, Bracewell³ defines the null function $\delta^0(x)$, which is nonzero at just a single point (see Figure 6a), as follows:

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

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 $x = \pm \frac{1}{2}$.

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

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:

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

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:

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

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:

$$e^{ix} = \cos(x) + i\sin(x) \quad (19)$$

and similarly:

$$e^{-ix} = \cos(x) - i\sin(x) \quad (20)$$

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:

$$F(s) = \int_{-\infty}^{\infty} f(x) (\cos(2\pi sx) - i\sin(2\pi sx)) dx \quad (21)$$

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

and Equation 9 as:

$$f(x) = \int_{-\infty}^{\infty} F(s) (\cos(2\pi sx) + i\sin(2\pi sx)) ds \quad (22)$$

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

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 show 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.

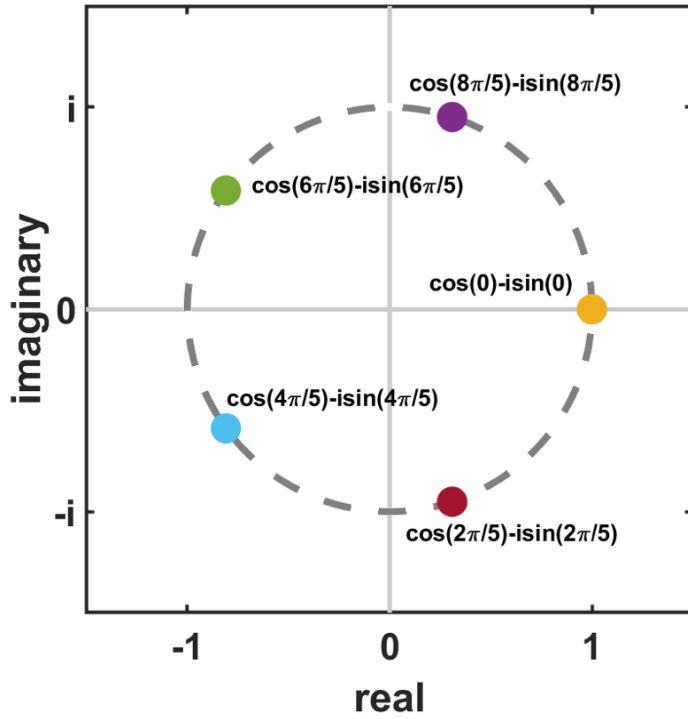


Figure 7. The five unique roots of unity for $e^{-i2\pi n/5}$.

2. Roots of unity

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:

$$e^{\pm i2\pi} = \cos(2\pi) \pm i\sin(2\pi) = \cos(2\pi) = 1, \quad (23)$$

and in addition, for n an integer:

$$e^{\pm i2\pi n} = \cos(2\pi n) \pm i\sin(2\pi n) = \cos(2\pi n) = 1 \quad (24)$$

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 $(e^{\pm i2\pi n/5})^5 = 1$ and $(e^{\pm i2\pi n/127})^{127} = 1$, 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, again, 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:

$$e^{-i2\pi 0/5} = \cos(0) - i\sin(0) = 1 \quad (25)$$

$$e^{-i2\pi 1/5} = \cos(2\pi/5) - i\sin(2\pi/5) \quad (26)$$

$$e^{-i2\pi 2/5} = \cos(4\pi/5) - i\sin(4\pi/5) \quad (27)$$

$$e^{-i2\pi 3/5} = \cos(6\pi/5) - i\sin(6\pi/5) \quad (28)$$

$$e^{-i2\pi 4/5} = \cos(8\pi/5) - i\sin(8\pi/5) \quad (29)$$

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.

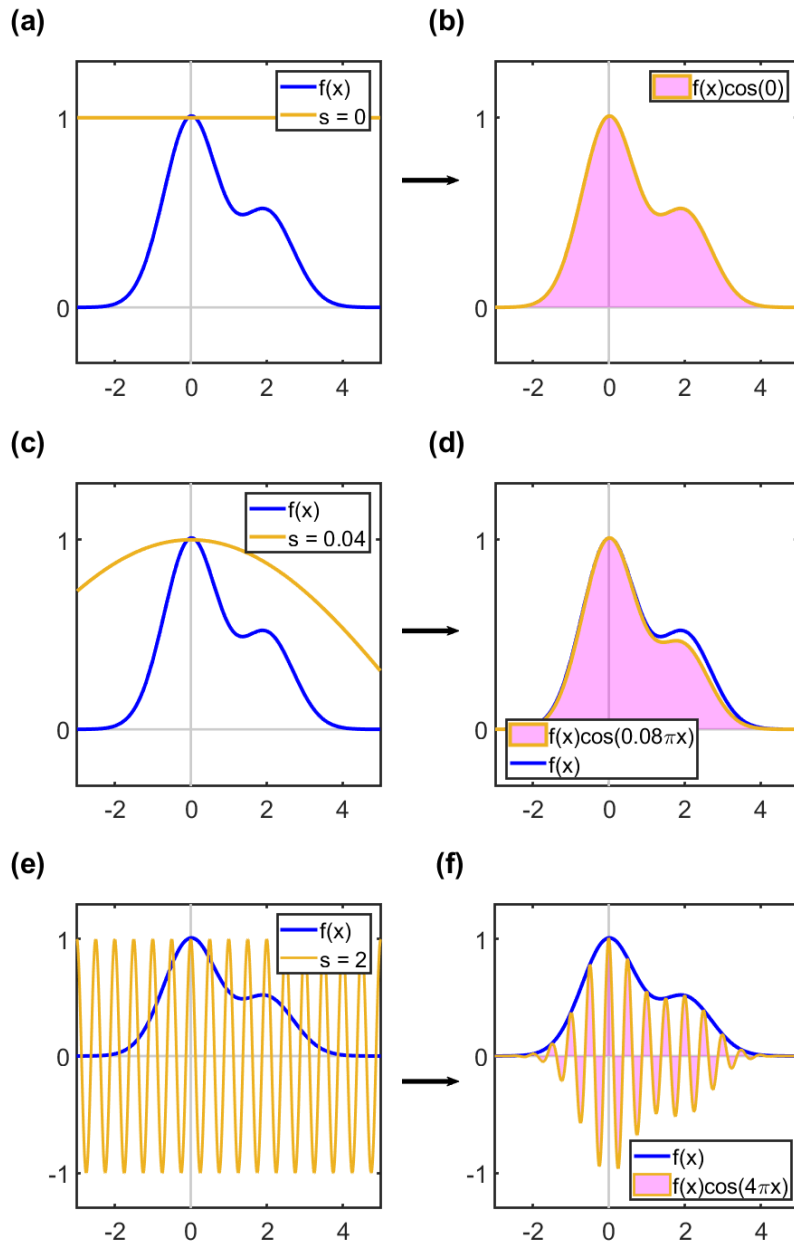


Figure 8. Graphical illustration of the Fourier transform of an arbitrary function, $f(x)$, for different values of s in $F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx} dx$ showing that (a – b) $F(0) = \int_{-\infty}^{\infty} f(x) dx$ and (c – f) suggesting that if $f(x)$ has finite support (it is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

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

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

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

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:

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

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 $s \rightarrow \pm\infty$, where we rewrite it as:

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

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 $s \rightarrow \pm\infty$ in $\cos(2\pi s x)$ and $\sin(2\pi s x)$ 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 $f(x) \cos(2\pi s x)$ and $f(x) \sin(2\pi s x)$, 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 $f(x) \cos(2\pi s x)$ in Figure 8e – f. This implies that for a continuous, well-behaved function with finite support $\lim_{s \rightarrow \pm\infty} F(s) = 0$.

D. *Even and odd functions*

1. *Introduction to 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 another 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). All odd functions that are defined at the origin must pass through the origin. Even functions can cross the y-axis at any point.

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.

2. *Unambiguously dividing an arbitrary function into its even and odd parts*

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

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

and

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

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:

$$f(x) = E_1(x) + O_1(x) \quad (35)$$

$$f(x) = E_2(x) + O_2(x) \quad (36)$$

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:

$$E_1(x) + O_1(x) = E_2(x) + O_2(x) \quad (37)$$

and with a little algebra we obtain:

$$E_1(x) - E_2(x) = O_2(x) - O_1(x) \quad (38)$$

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:

$$E_1(x) - E_2(x) = O_2(x) - O_1(x) = 0 \quad (39)$$

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.

3. *The areas of integrals of even and odd functions over symmetric limits*

From calculus we remember the following properties of even, $E(x)$, and odd, $O(x)$, functions in integrals, which follow directly from their symmetry:

$$\int_{-\infty}^{\infty} E(x)dx = 2 \int_0^{\infty} E(x)dx \quad (40)$$

and

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

These results can be proved fairly easily. To do so, we first write:

$$\int_{-a}^a E(x)dx = \int_{-a}^0 E(x)dx + \int_0^a E(x)dx \quad (42)$$

We now focus on the integral $\int_{-a}^0 E(x)dx$, where we change the variable in this integral to $x = -x'$, which leads to:

$$\begin{aligned} \int_{-a}^0 E(x)dx &= \int_a^0 E(-x')(-dx') \\ &= -\int_a^0 E(-x')dx' = \int_0^a E(-x')dx' = \int_0^a E(x')dx' = \int_0^a E(x)dx \end{aligned} \tag{43}$$

which allows us to write $\int_{-a}^a E(x)dx = 2 \int_0^a E(x)dx$ and therefore $\int_{-\infty}^{\infty} E(x)dx = 2 \int_0^{\infty} E(x)dx$ (when these improper integrals exist). The fact that $\int_{-\infty}^{\infty} O(x)dx = 0$ can be proved similarly.

4. *The integral of an arbitrary function over symmetric limits*

We now consider the integral over symmetric limits of an arbitrary function, $f(x)$, that has been decomposed into its even and odd parts: $f(x) = E(x) + O(x)$, as follows:

$$\begin{aligned} \int_{-a}^a f(x) dx &= \int_{-a}^a (E(x) + O(x)) dx \\ &= \int_{-a}^a E(x) dx + \int_{-a}^a O(x) dx = 2 \int_0^a E(x) dx \end{aligned} \tag{44}$$

Thus, in the integral of a function over symmetric limits, one can ignore the odd part of the function.

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.

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:

$$F_E(s) = \int_{-\infty}^{\infty} E(x) \cos(2\pi sx) dx - i \int_{-\infty}^{\infty} E(x) \sin(2\pi sx) dx \quad (45)$$

The integrand of the first integral in Equation 45 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 45 reduces to:

$$F_E(s) = 2 \int_0^{\infty} E(x) \cos(2\pi s x) dx \quad (46)$$

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

$$F_O(s) = \int_{-\infty}^{\infty} O(x) \cos(2\pi s x) dx - i \int_{-\infty}^{\infty} O(x) \sin(2\pi s x) dx \quad (47)$$

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

$$F_O(s) = -2i \int_0^{\infty} O(x) \sin(2\pi s x) dx \quad (48)$$

There is a delightful subtlety in Equations 46 and 48 that should not go unnoticed. First, in simplifying Equations 45 and 47 to get Equations 46 and 48, respectively, we used the fact that $E(x)$, $O(x)$, $\cos(2\pi s x)$, and $\sin(2\pi s x)$ 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 46 and 48 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 46, gives:

$$F_E(-s) = 2 \int_0^{\infty} E(x) \cos(-2\pi s x) dx = 2 \int_0^{\infty} E(x) \cos(2\pi s x) dx = F_E(s) \quad (49)$$

so $F_E(s)$ is even. Applying the same procedure for $F_O(s)$ in Equation 48, we obtain:

$$F_O(-s) = -2i \int_0^{\infty} O(x) \sin(-2\pi sx) dx = 2i \int_0^{\infty} O(x) \sin(2\pi sx) dx = -F_O(s) \quad (50)$$

so $F_O(s)$ is odd. That is, although the integrands of Equations 46 and 48 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.

$$\begin{aligned} F(s) &= \int_{-\infty}^{\infty} f(x) e^{-i2\pi sx} dx \\ &= \int_{-\infty}^{\infty} (E(x) + O(x)) e^{-i2\pi sx} dx \\ &= \int_{-\infty}^{\infty} (E(x) + O(x)) (\cos(2\pi sx) - i\sin(2\pi sx)) dx \end{aligned} \quad (51)$$

Multiplying the terms in the last equation of Equation 51 gives:

$$\begin{aligned}
& \int_{-\infty}^{\infty} E(x) \cos(2\pi s x) dx - i \int_{-\infty}^{\infty} E(x) \sin(2\pi s x) dx + \int_{-\infty}^{\infty} O(x) \cos(2\pi s x) dx \\
& - i \int_{-\infty}^{\infty} O(x) \sin(2\pi s x) dx
\end{aligned} \tag{52}$$

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 52 reduces to:

$$\int_{-\infty}^{\infty} E(x) \cos(2\pi s x) dx - i \int_{-\infty}^{\infty} O(x) \sin(2\pi s x) dx \tag{53}$$

As noted above, $\int_{-\infty}^{\infty} E(x) \cos(2\pi s x) dx$ is an even function and $\int_{-\infty}^{\infty} O(x) \sin(2\pi s x) dx$ 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.

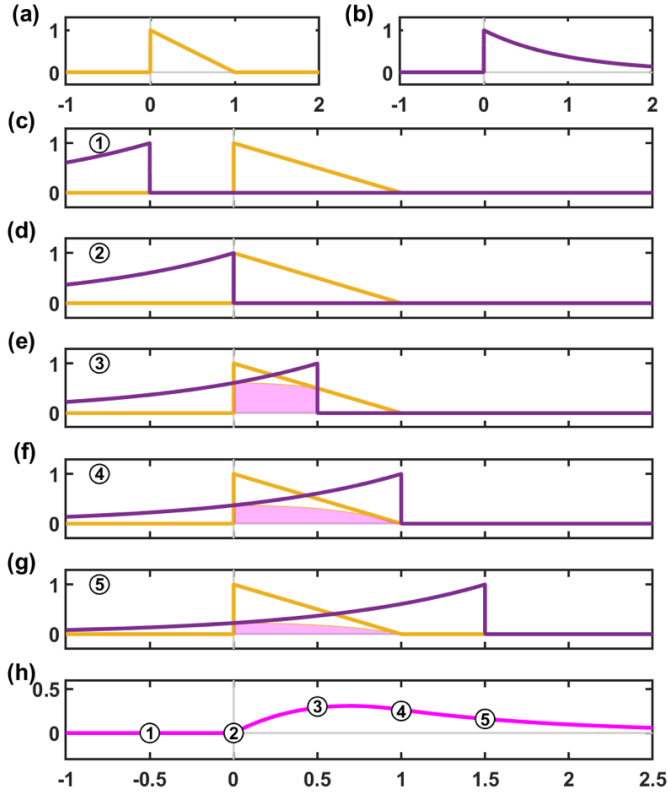


Figure 9. A graphical illustration of convolution. (a – b) Two functions to be convolved, where, in this convolution, the triangular function will remain unchanged, and the decaying exponential function will be reversed and shifted to various positions. (c – g) A graphical representation of the convolution between the functions in (a) and (b) where the decaying exponential function has been reversed and placed at different positions relative to the triangular function. (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:

$$h(x) = f(x) * g(x) = \int_{-\infty}^{\infty} f(\tau) g(x - \tau) d\tau \quad (54)$$

That is, when the functions we wish to convolve, $f(x)$ and $g(x)$, go into the convolution integral (Equation 54), 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:

$$f(x) * g(x) = g(x) * f(x) \quad (55)$$

As shown in Equation 56, this result can be proved in a few steps. First, in Equation 56, we change the variable in Equation 54 from τ to τ' by setting $\tau' = x - \tau$, 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 56, 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 56 is equal to $g(x) * f(x)$, which completes our proof.

$$\begin{aligned}
 h(x) = f(x) * g(x) &= \int_{-\infty}^{\infty} f(\tau) g(x - \tau) d\tau = \int_{\infty}^{-\infty} f(x - \tau') g(\tau') (-d\tau') \\
 &= \int_{-\infty}^{\infty} g(\tau) f(x - \tau) d\tau = g(x) * f(x)
 \end{aligned} \tag{56}$$

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*

As defined by different authors, the addition, sum, and/or linearity theorems are all quite similar. They basically state 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:

$$\begin{aligned}
 F(s) &= \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx} dx = \int_{-\infty}^{\infty} (ag(x) + bh(x))e^{-i2\pi sx} dx & (57) \\
 &= \int_{-\infty}^{\infty} ag(x)e^{-i2\pi sx} dx + \int_{-\infty}^{\infty} bh(x)e^{-i2\pi sx} dx \\
 &= a \int_{-\infty}^{\infty} g(x)e^{-i2\pi sx} dx + b \int_{-\infty}^{\infty} h(x)e^{-i2\pi sx} dx \\
 &= aG(s) + bH(s)
 \end{aligned}$$

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:

$$\int_{-\infty}^{\infty} f(x-a)e^{-i2\pi sx} dx \quad (58)$$

and then substitute in $x' = x - a$, which gives us:

$$\int_{-\infty}^{\infty} f(x')e^{-i2\pi s(x'+a)} dx' = \int_{-\infty}^{\infty} f(x')e^{-i2\pi sx'} e^{-i2\pi sa} dx' \quad (59)$$

The limits of integration stay 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 59, and also that x' is a dummy variable, we remove $e^{-i2\pi sa}$ from the integral and replace x' with x , writing:

$$e^{-i2\pi sa} \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx} dx = e^{-i2\pi sa} F(s) \quad (60)$$

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

$$\begin{aligned} \int_{-\infty}^{\infty} f(x+a)e^{-i2\pi sx} dx &= \int_{-\infty}^{\infty} f(x')e^{-i2\pi s(x'-a)} dx' \\ &= e^{i2\pi sa} \int_{-\infty}^{\infty} f(x')e^{-i2\pi sx'} dx' = e^{i2\pi sa} F(s) \end{aligned} \quad (61)$$

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 reveals that the convolution of two functions in one domain is equivalent to multiplication of their Fourier transforms in the other domain, i.e., $\mathcal{F}\{f(x) * g(x)\} = F(s)G(s)$ or, equivalently, $f(x) * g(x) = \mathcal{F}^{-1}\{F(s)G(s)\}$. This theorem often allows us to replace a computationally expensive convolution in direct space with a multiplication in reciprocal space. The importance of this theorem for data smoothing and data processing cannot be overstated.

We begin our proof of the convolution theorem by rewriting Equation 54, which defines the convolution of two functions, $f(x)$ and $g(x)$.

$$f(x) * g(x) = \int_{-\infty}^{\infty} f(\tau) g(x - \tau) d\tau \quad (62)$$

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

$$\mathcal{F}\{f(x) * g(x)\} = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} f(\tau) g(x - \tau) d\tau \right] e^{-i2\pi s x} dx \quad (63)$$

Reversing the order of integration gives us:

$$\mathcal{F}\{f(x) * g(x)\} = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} g(x - \tau) e^{-i2\pi s x} dx \right] f(\tau) d\tau \quad (64)$$

We use the shift theorem (Equations 59 and 60) to solve the inner integral in Equation 64, which gives us:

$$\mathcal{F}\{f(x) * g(x)\} = \int_{-\infty}^{\infty} [G(s)e^{-i2\pi s\tau}] f(\tau) d\tau \quad (65)$$

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

$$\mathcal{F}\{f(x) * g(x)\} = G(s) \int_{-\infty}^{\infty} f(\tau) e^{-i2\pi s\tau} d\tau = F(s)G(s) \quad (66)$$

Again, convolution itself, which, again, 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. 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 66 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. *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:

$$f(x) = \mathcal{F}^{-1}\{F(s)\} = \int_{-\infty}^{\infty} F(s) e^{i2\pi s x} ds \quad (67)$$

We first take the derivative of Equation 67:

$$\frac{df(x)}{dx} = \frac{d \mathcal{F}^{-1}\{F(s)\}}{dx} = \frac{d}{dx} \int_{-\infty}^{\infty} F(s) e^{i2\pi s x} ds \quad (68)$$

and then switch the order of differentiation and integration:

$$\begin{aligned} \frac{df(x)}{dx} &= \frac{d}{dx} \int_{-\infty}^{\infty} F(s) e^{i2\pi s x} ds = \int_{-\infty}^{\infty} F(s) \left(\frac{d}{dx} e^{i2\pi s x} \right) ds \\ &= \int_{-\infty}^{\infty} i2\pi s F(s) e^{i2\pi s x} ds \end{aligned} \quad (69)$$

Equations 68 and 69 are equivalent to writing $\mathcal{F}\left(\frac{df(x)}{dx}\right) = i2\pi s F(s)$, 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, $\frac{d^2f(x)}{dx^2}$, 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 $\frac{df(x)}{dx} = D^1 f$, $\frac{d^2f(x)}{dx^2} = D^2 f$, $\frac{d^n f(x)}{dx^n} = D^n f$, 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 obvious 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 together in our final result.

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

$$\mathcal{F}(f(ax)) = \int_{-\infty}^{\infty} f(ax) e^{-i2\pi s x} dx \quad (70)$$

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:

$$\begin{aligned} \int_{-\infty}^{\infty} f(ax) e^{-i2\pi sx} dx &= \int_{-\infty}^{\infty} f(x') e^{-i2\pi s\left(\frac{x'}{a}\right)} \frac{dx'}{a} = \int_{-\infty}^{\infty} f(x') e^{-i2\pi\left(\frac{s}{a}\right)x'} \frac{dx'}{a} \\ &= \frac{1}{a} \int_{-\infty}^{\infty} f(x') e^{-i2\pi\left(\frac{s}{a}\right)x'} dx' = \frac{1}{a} F\left(\frac{s}{a}\right) \end{aligned} \quad (71)$$

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

$$\mathcal{F}(f(ax)) = \int_{-\infty}^{\infty} f(ax) e^{-i2\pi sx} dx \quad (72)$$

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:

$$\begin{aligned} \int_{-\infty}^{\infty} f(ax) e^{-i2\pi sx} dx &= \int_{\infty}^{-\infty} f(x') e^{-i2\pi s\left(\frac{x'}{a}\right)} \frac{dx'}{a} = \frac{1}{a} \int_{\infty}^{-\infty} f(x') e^{-i2\pi\left(\frac{s}{a}\right)x'} dx' \\ &= -\frac{1}{a} \int_{-\infty}^{\infty} f(x') e^{-i2\pi\left(\frac{s}{a}\right)x'} dx' = -\frac{1}{a} F\left(\frac{s}{a}\right) \end{aligned} \quad (73)$$

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

$$\mathcal{F}(f(ax)) = \frac{1}{|a|} F\left(\frac{s}{a}\right) \quad (74)$$

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.

The similarity theorem allows us to quickly prove that if $F(s)$ is the Fourier transform of $f(x)$, then $F(-s)$ is the Fourier transform of $f(-x)$. We prove this by taking $a = -1$ in Equation 74. That is, for $\mathcal{F}(f(ax)) = \frac{1}{|a|} F\left(\frac{s}{a}\right)$, we have $\mathcal{F}(f(-x)) = \frac{1}{|-1|} F\left(\frac{s}{-1}\right) = \mathcal{F}(f(-x)) = F(-s)$.

8. Derivative of a Convolution Integral

This theorem says that for two functions, $f(x)$ and $g(x)$, $\frac{d}{dx}(f(x) * g(x)) = f'(x) * g(x) = f(x) * g'(x)$. 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 again that if $f(x)$ and $g(x)$ have Fourier transforms of $F(s)$ and $G(s)$, the convolution theorem tells us that $\mathcal{F}(f(x) * g(x)) = F(s)G(s)$. We next use the derivative theorem, which tells us that $\mathcal{F}\left(\frac{d}{dx}(f(x) * g(x))\right) = i2\pi s(F(s)G(s))$. Basic algebra and the convolution theorem then allow us to conclude that:

$$\mathcal{F}\left(\frac{d}{dx}(f(x) * g(x))\right) = i2\pi s(F(s)G(s)) = (i2\pi sF(s))G(s) \quad (75)$$

$$= \mathcal{F}(f'(x) * g(x)) = F(s)(i2\pi sG(s)) = \mathcal{F}(f(x) * g'(x))$$

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

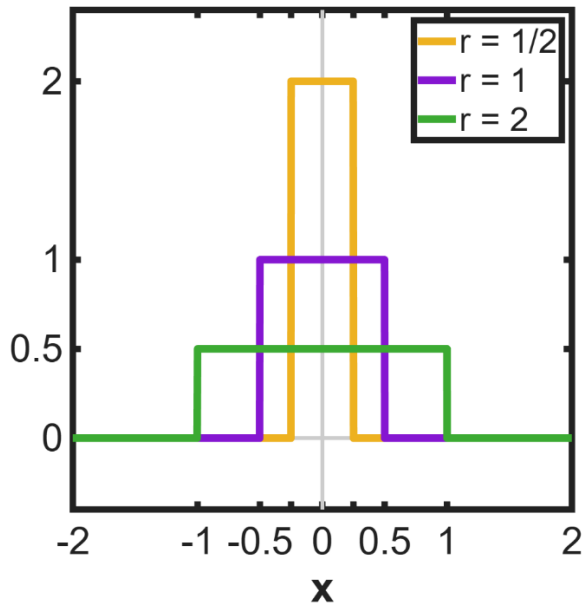


Figure 10. The boxcar function, $\frac{1}{r}\Pi\left(\frac{x}{r}\right)$, for $r = \frac{1}{2}, 1$, and 2 .

H. The impulse (delta) function

1. Definition of the delta function

The impulse function, or delta function, is defined as

$$\delta(x) = 0 \text{ for } x \neq 0 \quad (76)$$

and

$$\int_{-\infty}^{\infty} \delta(x) dx = 1 \quad (77)$$

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. There is no real function that has the properties of the delta function. However, there are infinitely many approximating sequences of functions that can be defined to meet the conditions outlined in Equations 76 and 77. Technically speaking, the delta function is referred to as a generalized function.

2. *Creating a delta function from the boxcar function*

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 $r \rightarrow 0$, we obtain a null function:

$$\delta^0(x) = \lim_{r \rightarrow 0} \Pi\left(\frac{x}{r}\right) \quad (78)$$

We can confirm that we have a null function by integrating Equation 78, which gives:

$$\int_{-\infty}^{\infty} \lim_{r \rightarrow 0} \Pi\left(\frac{x}{r}\right) dx = \lim_{r \rightarrow 0} \int_{-\frac{r}{2}}^{\frac{r}{2}} 1 dx = \lim_{r \rightarrow 0} r = 0 \quad (79)$$

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:

$$\delta(x) = \lim_{r \rightarrow 0} \frac{1}{r} \Pi\left(\frac{x}{r}\right) \quad (80)$$

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 .

3. *Properties of the delta function*

As defined in Equations 76 – 77, 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. Indeed, it is best understood when it is in an integral. The delta function picks out a value of the function that is in an integral. Let's first consider:

$$\int_{-\infty}^{\infty} \delta(x) f(x) dx \quad (81)$$

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:

$$\int_{-\infty}^{\infty} \delta(x) f(x) dx = \int_{-\infty}^{\infty} \delta(x) f(0) dx \quad (82)$$

Furthermore, $f(x)$ approaches the constant value of $f(0)$ as $x \rightarrow 0$, 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:

$$\int_{-\infty}^{\infty} \delta(x) f(x) dx = \int_{-\infty}^{\infty} \delta(x) f(0) dx = f(0) \int_{-\infty}^{\infty} \delta(x) dx = f(0) \quad (83)$$

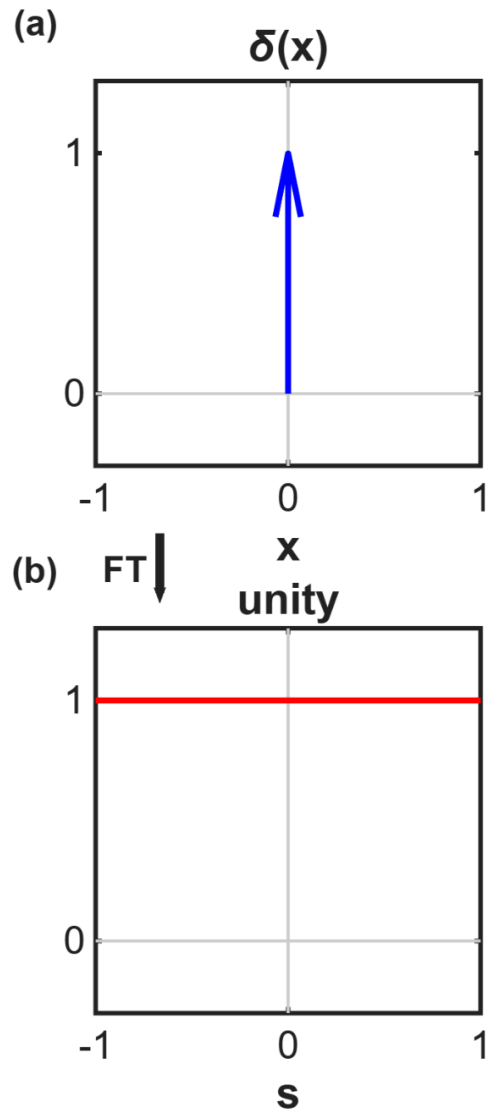


Figure 11. (a) Representation of the delta function, $\delta(x)$, and (b) its Fourier transform, which is unity. Note that in (a), the y-axis scale refers to the area of the delta function, not its height! The delta function is often represented as a spike, as in (a).

4. Fourier transform of the delta function

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

$$\int_{-\infty}^{\infty} \delta(x) e^{-i2\pi s x} dx = e^0 \int_{-\infty}^{\infty} \delta(x) dx = 1 \quad (84)$$

In other words, $\mathcal{F}(\delta(x)) = 1$ (see Figure 11). Similarly, recognizing that $\delta(x - a)$ is only nonzero at $x = a$, which makes the argument of the delta function zero, we can find the Fourier transform of a shifted delta function, $\delta(x - a)$, as follows:

$$F(s) = \int_{-\infty}^{\infty} \delta(x - a) e^{-i2\pi s x} dx = e^{-i2\pi s a} \int_{-\infty}^{\infty} \delta(x) dx = e^{-i2\pi s a} \quad (85)$$

Again, in an integral, the delta function picks out the value of the function at the point where it 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.

5. *The delta function in convolution*

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:

$$\delta(x) * f(x) = \int_{-\infty}^{\infty} \delta(\tau) f(x - \tau) d\tau = f(x) \int_{-\infty}^{\infty} \delta(\tau) d\tau = f(x) \quad (86)$$

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 important case of the convolution of a function with a shifted delta function, $\delta(x - a)$:

$$\begin{aligned}
 \delta(x - a) * f(x) & \qquad \qquad \qquad (87) \\
 &= \int_{-\infty}^{\infty} \delta(\tau - a) f(x - \tau) d\tau \\
 &= f(x - a) \int_{-\infty}^{\infty} \delta(\tau - a) d\tau = f(x - a)
 \end{aligned}$$

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.

6. *Properties of $\delta(ax)$*

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

$$\delta(x) = \frac{1}{|a|} \delta(ax) \qquad (88)$$

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

$$\int_{-\infty}^{\infty} \delta(x) dx = \int_{-\infty}^{\infty} \lim_{r \rightarrow 0} \frac{1}{r} \Pi\left(\frac{x}{r}\right) dx \quad (89)$$

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

$$\int_{-\infty}^{\infty} \delta(ax) dx = \int_{-\infty}^{\infty} \lim_{r \rightarrow 0} \frac{1}{r} \Pi\left(\frac{ax}{r}\right) dx \quad (90)$$

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 $a > 0$:

$$\begin{aligned} \int_{-\infty}^{\infty} \delta(ax) dx &= \int_{-\infty}^{\infty} \lim_{r \rightarrow 0} \frac{1}{r} \Pi\left(\frac{x'}{r}\right) \frac{dx'}{a} = \int_{-\infty}^{\infty} \left(\frac{1}{a}\right) \lim_{r \rightarrow 0} \frac{1}{r} \Pi\left(\frac{x'}{r}\right) dx' \\ &= \int_{-\infty}^{\infty} \frac{1}{a} \cdot \delta(x) dx \end{aligned} \quad (91)$$

For $a < 0$, we again substitute $x' = ax$ into Equation 90, which means that $dx' = adx$, and the limits of the integral are reversed:

$$\begin{aligned}
\int_{-\infty}^{\infty} \delta(ax) dx &= \int_{-\infty}^{\infty} \lim_{r \rightarrow 0} \frac{1}{r} \Pi\left(\frac{x'}{r}\right) \frac{dx'}{a} = \left(-\frac{1}{a}\right) \int_{-\infty}^{\infty} \lim_{r \rightarrow 0} \frac{1}{r} \Pi\left(\frac{x'}{r}\right) dx' \\
&= \int_{-\infty}^{\infty} -\frac{1}{a} \cdot \delta(x) dx
\end{aligned} \tag{92}$$

The results in the integrals in Equations 91 and 92 thus imply that $\delta(ax) = \frac{1}{|a|} \delta(x)$.

7. *Properties of $\delta(f(x))$*

We now consider the more advanced case of the argument of the delta function being another function: $\delta(f(x))$. Admittedly, this may appear a little strange. However, moving forward with an analysis of it, we note that it seems reasonable that $\delta(f(x))$ will have nonzero values only at the roots of $f(x)$, i.e., where it is zero. Accordingly, we assume that $f(x)$ has i isolated roots a_i . In addition, because the delta function is best understood in an integral – it is defined by an integral, we consider for another function $g(x)$:

$$\int_{-\infty}^{\infty} g(x) \delta(f(x)) dx = \sum_i \int_{a_i - \varepsilon}^{a_i + \varepsilon} g(x) \delta(f(x)) dx \tag{93}$$

where ε is a small number. That is, in Equation 93 we split up the original integral into small neighborhoods around the roots of $f(x)$. Now, very close to a root a_i of $f(x)$, $f(x) \approx f(a_i) + f'(a_i)(x - a_i)$, which is a Taylor series expansion of $f(x)$ around a_i . Now, by definition of a_i

being a root of $f(x)$, $f(a_i) = 0$, which gives us $f(x) \approx f'(a_i)(x - a_i)$. Thus, Equation 93 becomes:

$$\sum_i \int_{a_i-\varepsilon}^{a_i+\varepsilon} g(x) \delta(f'(a_i)(x - a_i)) dx \quad (94)$$

However, $f'(a_i)$ is just a number, which means we can invoke the result we just derived of $\delta(ax) = \frac{1}{|a|} \delta(x)$ and write:

$$\sum_i \int_{a_i-\varepsilon}^{a_i+\varepsilon} g(x) \delta(f'(a_i)(x - a_i)) dx = \sum_i \frac{g(a_i)}{|f'(a_i)|} \quad (95)$$

where we require that $|f'(a_i)| \neq 0$, i.e., the roots are simple.

8. *Defining the delta function asymmetrically so no ‘action’ takes place before a certain time*

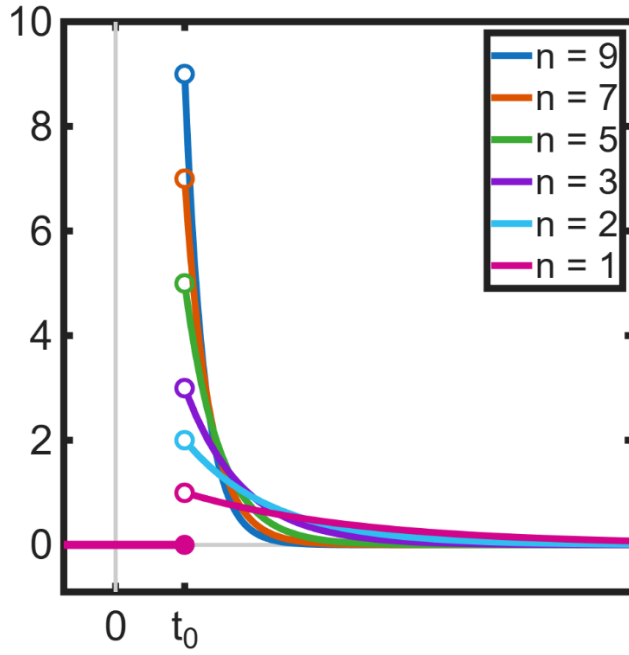


Figure 12. The delta function defined in Equation 96 for various values of n . This delta function precludes any action from taking place before t_0 .

Boas³⁹ presents two delta functions that do not allow any action prior to a starting time, t_0 . In this way, they are different from the delta function defined above (Equation 80), which is based on a series of boxcar function that are symmetric about the origin. Equation 96 defines the first of Boas' delta functions:

$$f_n(t) = \begin{cases} ne^{-n(t-t_0)}, & t > t_0 \\ 0, & t \leq t_0 \end{cases} \quad (96)$$

where this function is plotted in Figure 12 for $n = 1, 2, 3, 5, 7$, and 9 . Note that, as shown in the figure, $ne^{-n(t-t_0)} \rightarrow n$ as $t \rightarrow t_0$.

To show that $f_n(t)$ has the properties of a delta function, we first confirm that its integral is unity, as follows:

$$\begin{aligned}
\int_{t_0+\varepsilon}^{\infty} f_n(t) dt &= \int_{t_0+\varepsilon}^{\infty} n e^{-n(t-t_0)} dt & (97) \\
&= n e^{nt_0} \int_{t_0+\varepsilon}^{\infty} e^{-nt} dt = n e^{nt_0} \left(\frac{-1}{n} \right) e^{-nt} \Big|_{t_0+\varepsilon}^{\infty} \\
&= -n e^{nt_0} \left(\frac{-1}{n} \right) e^{-n(t_0+\varepsilon)} = e^{nt_0} e^{-n(t_0+\varepsilon)} = 1
\end{aligned}$$

where ε is a small number and we allow $\varepsilon \rightarrow 0$ at the end of the integral. Additionally, we note that for any $t > t_0$, $t - t_0 > 0$. Thus, $n e^{-n(t-t_0)}$ becomes $\frac{n}{e^{n(t-t_0)}}$, which has the form $\frac{\infty}{\infty}$ as $n \rightarrow \infty$. Accordingly, by L'Hôpital's rule, $\frac{n}{e^{n(t-t_0)}}$ becomes $\frac{1}{(t-t_0)e^{n(t-t_0)}}$, which means that $f_n(t) \rightarrow 0$ as $n \rightarrow \infty$ for, again, $t - t_0 > 0$. Also, for $t \rightarrow t_0$, $f_n(t) \rightarrow \infty$ as $n \rightarrow \infty$. Thus, the sequence of equations implied in Equation 96 satisfy the conditions for a delta function.

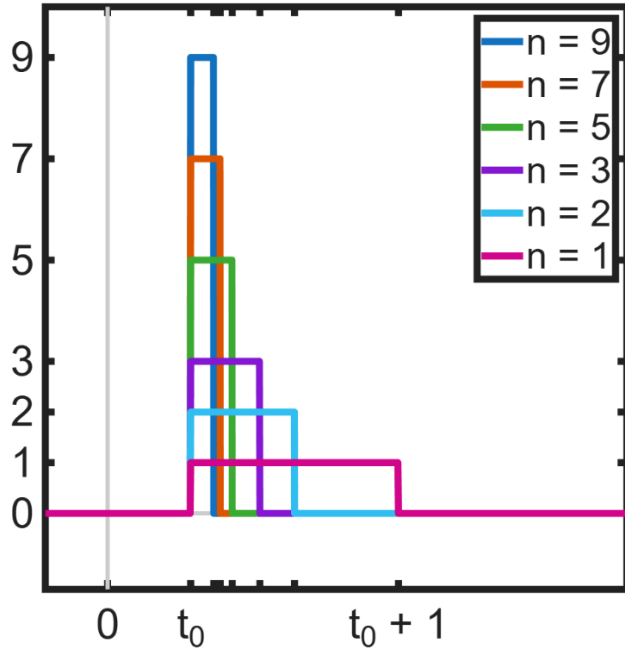


Figure 13. A delta function (Equation 98) that does not allow ‘action’ before a time t_0 .

Boas’ second delta function that does not allow ‘action’ before a certain time, t_0 , is:

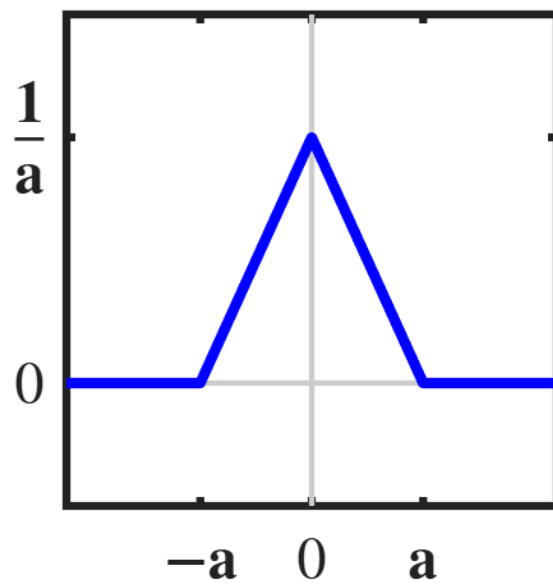
$$f_n(t) = \begin{cases} n, & t_0 < t < t_0 + \frac{1}{n} \\ 0, & \text{otherwise} \end{cases} \quad (98)$$

This simpler function is shown in Figure 13 for various values of n . Clearly, as $n \rightarrow \infty$ the area of $f_n(t)$ remains unity (we have $n \cdot \frac{1}{n}$), it becomes infinitely narrow, and its height goes to infinity, so we again have a delta function.

9. Other definitions of the delta function

Delta functions can also be defined from, for example, triangle, Gaussian, and Lorentzian functions, where these functions are discussed/mentioned below. Indeed, 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. Figure 14a shows a delta function defined in terms of a triangle function. That is, this figure shows a triangle with a base extending from $-a$ to a and a height centered at the origin of $1/a$. Obviously, the area of this function is unity. Accordingly, as $a \rightarrow 0$ this function becomes a delta function. Figure 14b shows the derivative of this function.

(a)



(b)

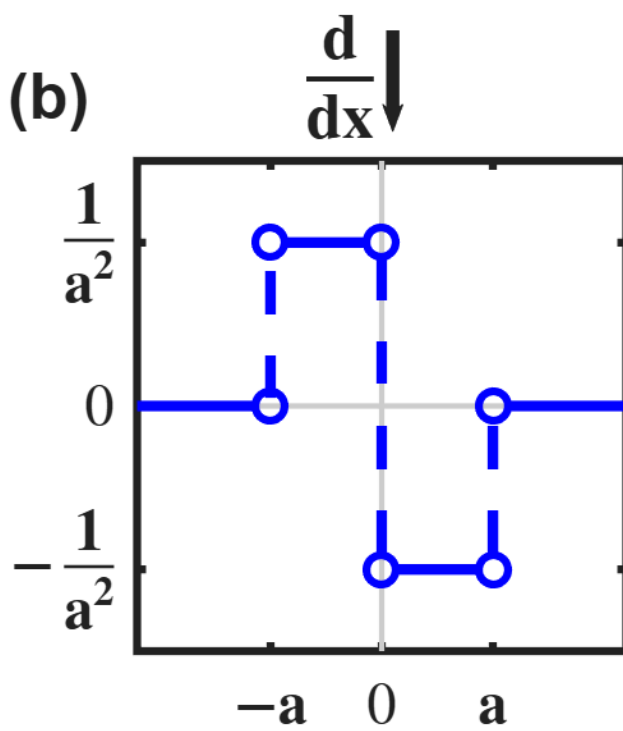


Figure 14. (a) The delta function defined in terms of a triangle function, where $a \rightarrow 0$, and (b) the derivative of the triangle function in (a).

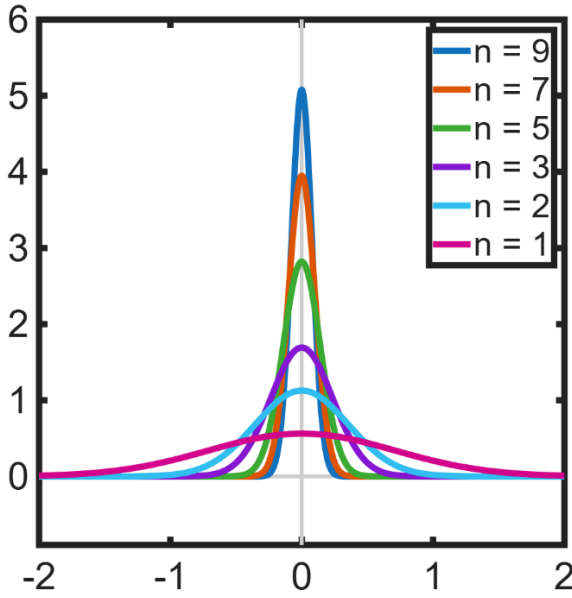


Figure 15. The delta function defined as a Gaussian (as in Equation 99) for various values of n .

Arfken and Weber⁴⁰ define the delta function in terms of a series of Gaussians with a parameter $n \rightarrow \infty$ as:

$$\delta_{n,Gaussian}(x) = \frac{n}{\sqrt{\pi}} e^{-n^2 x^2} \quad (99)$$

Figure 15 shows this function plotted for a few values of n . From a basic table of integrals, we know that $\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$. Based on this fact, it can be shown that $\int_{-\infty}^{\infty} \frac{n}{\sqrt{\pi}} e^{-n^2 x^2} dx = 1$. Furthermore, as $n \rightarrow \infty$, $\frac{n}{\sqrt{\pi}} e^{-n^2 x^2}$ becomes infinitely narrow and tall, i.e., in the limit this function is a delta function.

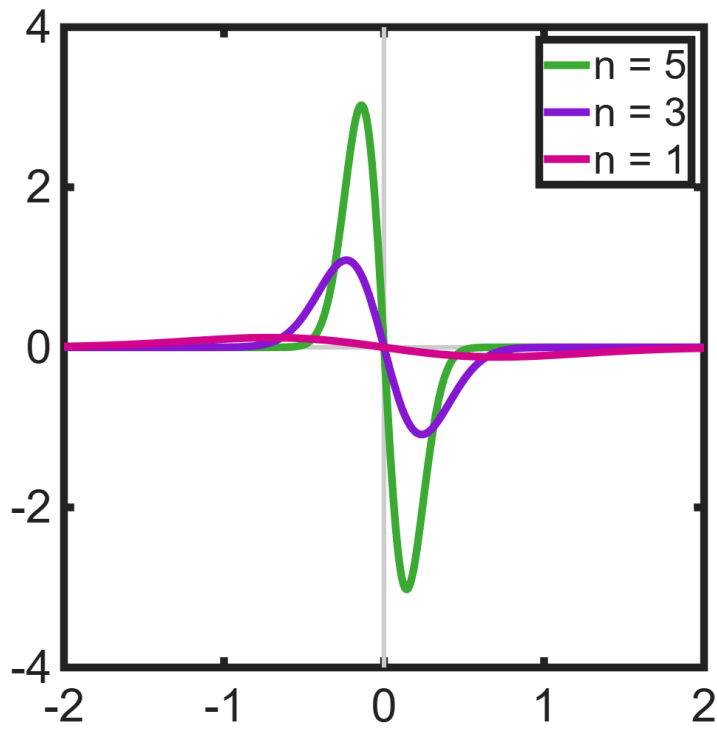


Figure 16. Derivatives of the delta function defined in Equation 99 for three values of n .

Figure 16 shows derivatives of the Gaussian in Equation 99 for three values of n . As $n \rightarrow \infty$, the derivative of Equation 99 functions as the derivative of the delta function.

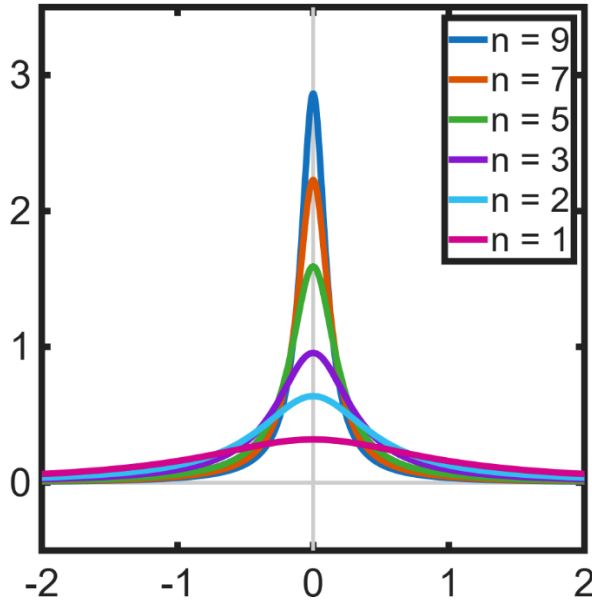


Figure 17. The delta function defined as a Lorentzian (as in Equation 99) for various values of n .

Arfken and Weber⁴⁰ also define the delta function as a Lorentzian, as follows:

$$\delta_{n,Lorentzian}(x) = \frac{n}{\pi} \cdot \frac{1}{1+n^2x^2} \quad (100)$$

Figure 17 shows this function plotted with a few values of n . The improper integral $\int_{-\infty}^{\infty} \frac{1}{1+x^2} dx = \pi$, which can be found in a table of integrals, can be used to show that $\int_{-\infty}^{\infty} \frac{n}{\pi} \cdot \frac{1}{1+n^2x^2} dx = 1$. In addition, at $x = 0$, $\frac{n}{\pi} \cdot \frac{1}{1+n^2x^2} \rightarrow \infty$ as $n \rightarrow \infty$. For $x \neq 0$, $\frac{n}{\pi} \cdot \frac{1}{1+n^2x^2} \rightarrow 0$ as $n \rightarrow \infty$, by, say, L'Hôpital's rule.

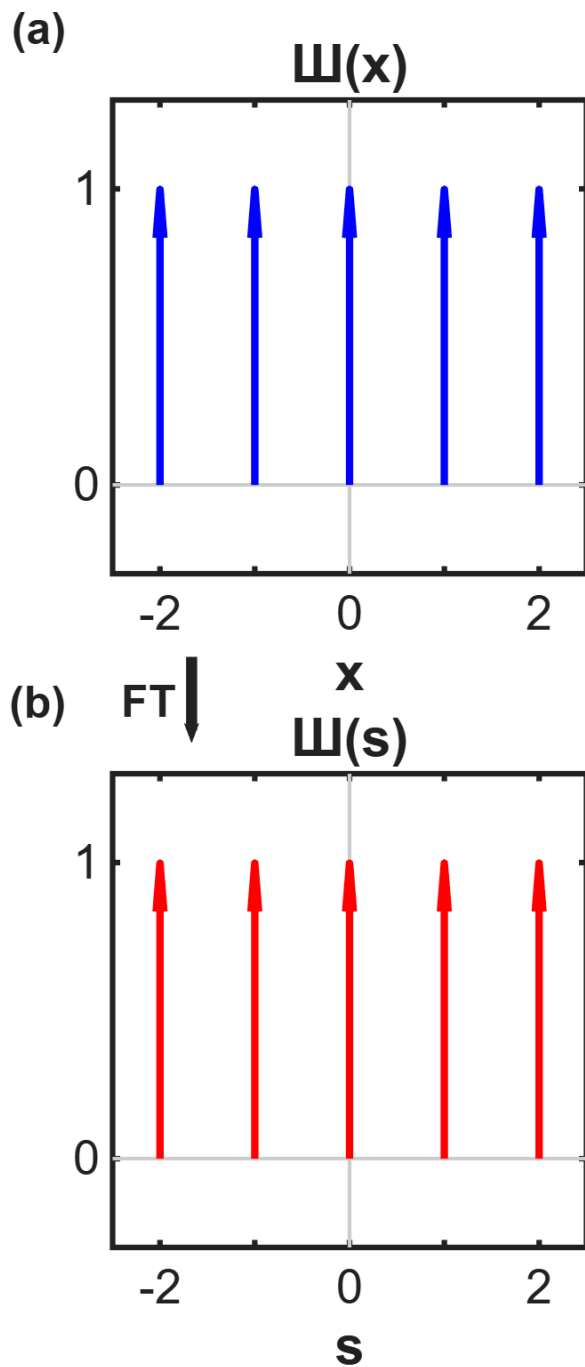


Figure 18. (a) The central part of the shah function in direct space, $\mathbb{W}(x)$, and (b) the central part of its Fourier transform $\mathbb{W}(s)$.

I. The shah (comb) function

The shah function, $\mathbb{I}\mathbb{I}(x)$, which is shown in Figure 18, is an infinite set of delta functions spaced at unit intervals across the x-axis, as follows:

$$\mathbb{I}\mathbb{I}(x) = \sum_{n=-\infty}^{\infty} \delta(x - n) \quad (101)$$

where n is an integer. The symbol for this function, $\mathbb{I}\mathbb{I}$, has Cyrillic roots, which relates it to the Hebrew letter ϖ (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 $\mathbb{I}\mathbb{I}$ are meant to resemble a series of delta functions, where, again, 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, $\mathbb{I}\mathbb{I}(x)f(x)$, as follows:

$$\begin{aligned} \mathbb{I}\mathbb{I}(x)f(x) &= \left(\sum_{n=-\infty}^{\infty} \delta(x - n) \right) f(x) \\ &= \sum_{n=-\infty}^{\infty} f(x)\delta(x - n) = \sum_{n=-\infty}^{\infty} f(n)\delta(x - n) \end{aligned} \quad (102)$$

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 $\mathbb{I}\mathbb{I}(ax)$. From the theory developed in this document we can write:

$$\mathbb{I}\mathbb{I}(ax) = \sum_{n=-\infty}^{\infty} \delta(ax - n) = \sum_{n=-\infty}^{\infty} \delta\left(a\left(x - \frac{n}{a}\right)\right) = \frac{1}{|a|} \sum_{n=-\infty}^{\infty} \delta\left(x - \frac{n}{a}\right) \quad (103)$$

Thus, by changing a in $\text{III}(ax)$, we change the spacing between the delta functions in our $\text{III}(ax)$ function compared to $\text{III}(x)$, 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.

$$f(x) * \text{III}(ax) = f(x) \tag{104}$$

$$\begin{aligned} & * \sum_{n=-\infty}^{\infty} \frac{1}{|a|} \delta\left(x - \frac{n}{a}\right) \\ &= \sum_{n=-\infty}^{\infty} f(x) * \frac{1}{|a|} \delta\left(x - \frac{n}{a}\right) = \frac{1}{|a|} \sum_{n=-\infty}^{\infty} f\left(x - \frac{n}{a}\right) \end{aligned}$$

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 replicated copies of a function may overlap.

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

$$\Pi_c(x) = \begin{cases} 0, & \text{for } x \leq -\frac{1}{2} \\ 1, & \text{for } -\frac{1}{2} < x \leq \frac{1}{2} \\ 0, & \text{for } x > \frac{1}{2} \end{cases} \tag{105}$$

where we now note that $\text{III}(x) * \Pi_c(x) = 1$.

Of course,

$$\int_{n^{-1/2}}^{n^{+1/2}} \text{III}(x) dx = 1, \text{ for all integers } n \quad (106)$$

More thoroughly, we could write:

$$\int_{n-a}^{n+a} \text{III}(x) dx = 1, \text{ for all integers } n \text{ and } 0 < a < 1 \quad (107)$$

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

J. Some common Fourier transform pairs

1. Initial Comments

The following transform pairs, i.e., a function and its Fourier transform, are important in Fourier theory. We will denote a Fourier transform pair in this section, and later in this work, with a double-headed arrow: ‘ $\leftrightarrow$ ’. However, even though this list may appear to show that there are quite a few Fourier transform pairs, we again emphasize that there are relatively few functions that can be easily Fourier transformed and/or that have nice, simple Fourier transforms.

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, $E(x)$:

$$\int_{-\infty}^{\infty} E(x) e^{-i2\pi s x} dx = \int_{-\infty}^{\infty} E(x) e^{i2\pi s x} dx = \int_{-\infty}^{\infty} E(x) \cos(2\pi s x) dx \quad (108)$$

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

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

$$\int_{-\infty}^{\infty} e_{direct}(x) e^{-i2\pi s x} dx = E_{reciprocal}(s) \quad (109)$$

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

$$e_{direct}(x) = \int_{-\infty}^{\infty} E_{reciprocal}(s) e^{i2\pi sx} ds \quad (110)$$

But it doesn't matter what we call x and s in Equation 110, so we can switch x and s to obtain:

$$e_{direct}(s) = \int_{-\infty}^{\infty} E_{reciprocal}(x) e^{i2\pi sx} dx \quad (111)$$

Equation 108 then allows us to write:

$$e_{direct}(s) = \int_{-\infty}^{\infty} E_{reciprocal}(x) e^{-i2\pi sx} dx \quad (112)$$

Thus, we see that:

$$\text{If } e_{direct}(x) \leftrightarrow E_{reciprocal}(s) \text{ then } E_{reciprocal}(x) \leftrightarrow e_{direct}(s). \quad (113)$$

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

We bring up this fact because a number of the Fourier transform pairs discussed below involve even functions. Thus, by Equation 113 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 $\Pi(x) \leftrightarrow \text{sinc}(s)$ was discussed above. It is shown in Figure 5. From Equation 113, it is also true that $\text{sinc}(x) \leftrightarrow \Pi(s)$. We will not repeat this relationship for the transform pairs of the other even functions below. Note that the Fourier transform of $\text{sinc}(x)$, which is $\Pi(s)$, is non-zero only over a limited set of frequencies. Functions with this property are said to be ‘band-limited’.

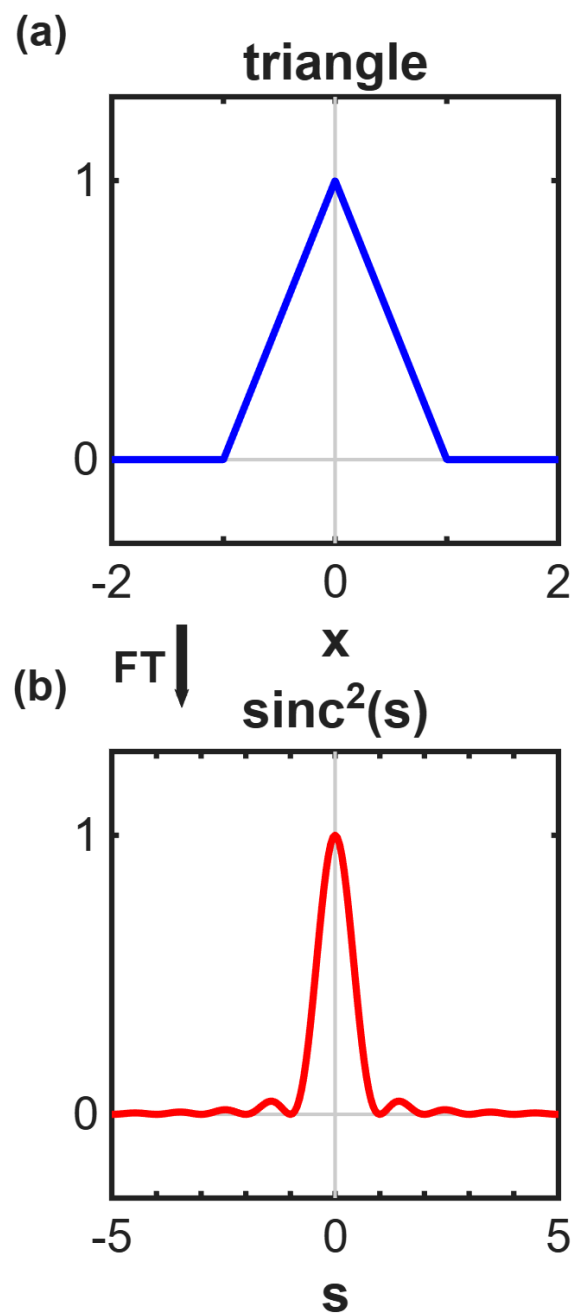


Figure 19. (a) The triangle function, $\Lambda(x)$, and (b) its Fourier transform $\text{sinc}^2(s)$.

4. The triangle function-sinc² pair

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

$$\Lambda(x) = \begin{cases} 1 - |x|, & |x| \leq 1 \\ 0, & |x| > 1 \end{cases} \quad (114)$$

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 function. 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, $\mathcal{F}(\Lambda(x)) = \mathcal{F}(\Pi(x) * \Pi(x)) = \text{sinc}(s) \cdot \text{sinc}(s) = \text{sinc}^2(s)$. The transform pair $\Lambda(x) \leftrightarrow \text{sinc}^2(s)$ is shown in Figure 19.

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:

$$F(s) = \int_{-\infty}^{\infty} 1 \cdot e^{-i2\pi sx} dx \quad (115)$$

We then note that, under these symmetric limits (from $-\infty$ to ∞), all the sine components of $e^{-i2\pi sx}$ are zero. Thus, Equation 115 becomes:

$$F(s) = \int_{-\infty}^{\infty} 1 \cdot \cos(2\pi sx) dx \quad (116)$$

We now consider two scenarios for Equation 116. In the first case, $s = 0$, which gives:

$$F(0) = \int_{-\infty}^{\infty} 1 dx \quad (117)$$

which implies that $F(0)$ is infinity. In the second case, we consider $s \neq 0$. Technically speaking, Equation 116 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. Considering these two cases creates a plausibility argument for $1 \leftrightarrow \delta(s)$.

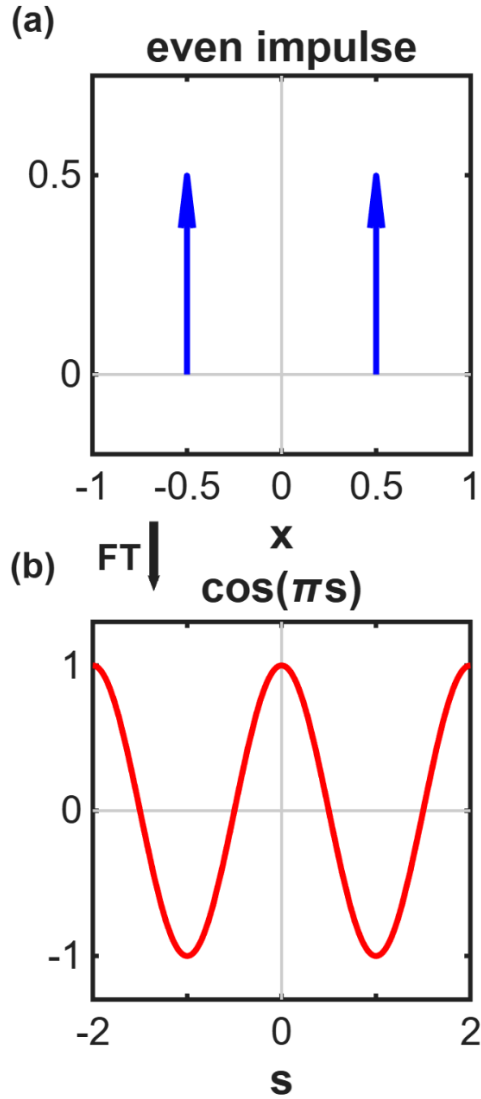


Figure 20. The (a) Even impulse pair: $II(x) = \frac{1}{2} \left(\delta \left(x + \frac{1}{2} \right) + \delta \left(x - \frac{1}{2} \right) \right)$, and (b) Cosine ($\cos(\pi s)$) Fourier transform pair.

We previously noted that the delta function acts as the identity for convolution, i.e., $\delta(x) * f(x) = f(x)$. Certainly, then we would then expect that $\delta(x) * \delta(x) = \delta(x)$. However, now that we have the transform pair $\delta(x) \leftrightarrow 1$, we can use the convolution theorem to further confirm this result. That is, from the convolution theorem, we can write that $\mathcal{F}\{\delta(x) * \delta(x)\} = 1 \cdot 1 = 1$, or $\mathcal{F}^{-1}\{1\} = \delta(x) * \delta(x)$, but we also know that $\mathcal{F}^{-1}\{1\} = \delta(x)$ so $\delta(x) * \delta(x) = \delta(x)$.

6. Even impulse pair-Cosine pair

Consider the Fourier transform of the following function of two delta functions:

$\frac{1}{2}(\delta(x + a) + \delta(x - a))$, where a is a real number:

$$\frac{1}{2} \int_{-\infty}^{\infty} (\delta(x + a) + \delta(x - a)) e^{-i2\pi s x} dx = \frac{1}{2} (e^{i2\pi s a} + e^{-i2\pi s a}) = \cos(2\pi s a) \quad (118)$$

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.

Bracewell³ defines the $\Pi(x)$ function as $\frac{1}{2}(\delta(x + \frac{1}{2}) + \delta(x - \frac{1}{2}))$, which, per Equation 118, has a Fourier transform of $\cos(\pi s)$ (see Figure 20). This symbol (Π) is obviously supposed to be reminiscent of a pair of delta functions.

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

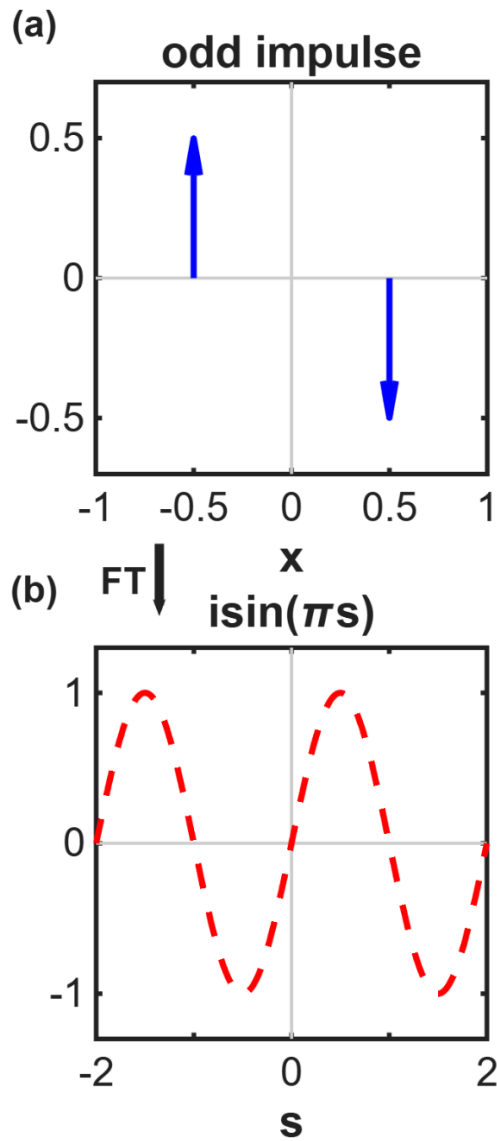


Figure 21.(a) The odd impulse pair $I_I(x) = \frac{1}{2} \left(\delta \left(x + \frac{1}{2} \right) - \delta \left(x - \frac{1}{2} \right) \right)$ and (b) its Fourier transform $i\sin(2\pi as)$. The dashed line reminds us that the function in (b) is imaginary.

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:

$$\frac{1}{2} \int_{-\infty}^{\infty} (\delta(x+a) - \delta(x-a)) e^{-i2\pi s x} dx = \frac{1}{2} (e^{i2\pi s a} - e^{-i2\pi s a}) = i \sin(2\pi s a) \quad (119)$$

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, $\frac{1}{2}(\delta(x+a) - \delta(x-a))$, is an imaginary odd function.

Bracewell³ defines the function $I_I(x)$ as $\frac{1}{2}(\delta(x + \frac{1}{2}) - \delta(x - \frac{1}{2}))$, which has a Fourier transform of $i \sin(\pi s)$ (see Figure 21). This symbol (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, $\frac{1}{2}(\delta(x+a) - \delta(x-a)) \leftrightarrow i \sin(2\pi s a)$, and $I_I(x) = \frac{1}{2}(\delta(x + \frac{1}{2}) - \delta(x - \frac{1}{2})) \leftrightarrow i \sin(\pi s)$, 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 in the following discussion because of Lerch's theorem. That is, it is true that $\delta^0(t)$ is an even function and that $\mathcal{F}(\delta^0(t)) = 0$, 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 (a.e.).

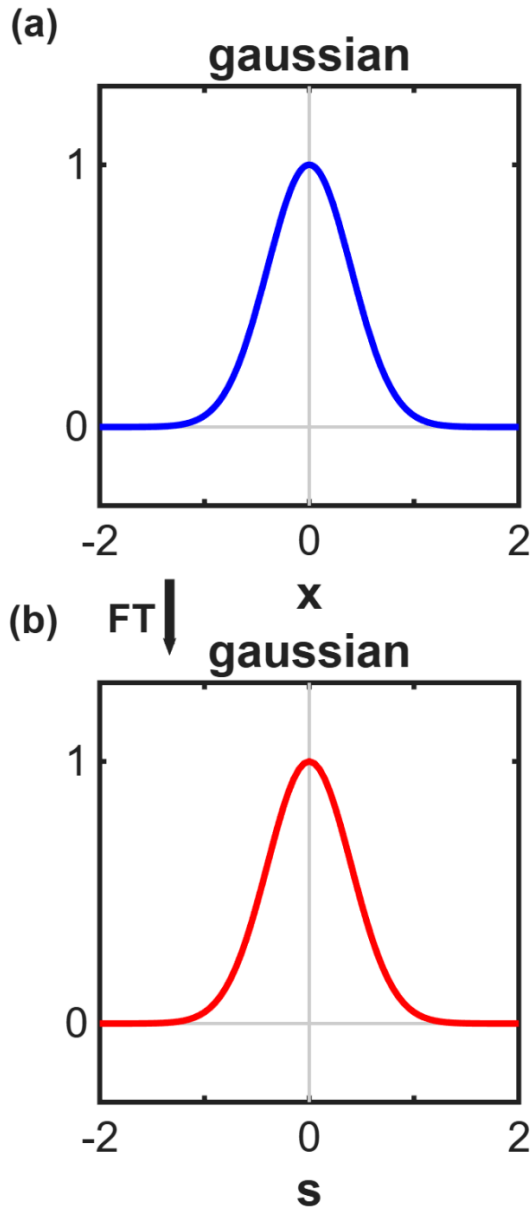


Figure 22. (a) The Gaussian $e^{-\pi x^2}$ in direct space, and (b) the Gaussian $e^{-\pi s^2}$ in reciprocal space as a Fourier transform pair.

9. The Gaussian-Gaussian pair

An important Fourier transform pair is $e^{-\pi x^2} \leftrightarrow e^{-\pi s^2}$, see Figure 22, which we obtain as follows. First, we write out the Fourier transform for $e^{-\pi x^2}$, which is:

$$\int_{-\infty}^{\infty} e^{-\pi x^2} e^{-i2\pi s x} dx \quad (120)$$

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

$$\int_{-\infty}^{\infty} e^{-\pi x^2} \cos(2\pi s x) dx \quad (121)$$

Equation 121 can be looked up in a table of integrals and is $e^{-\pi s^2}$. Thus, $e^{-\pi x^2} \leftrightarrow e^{-\pi s^2}$.

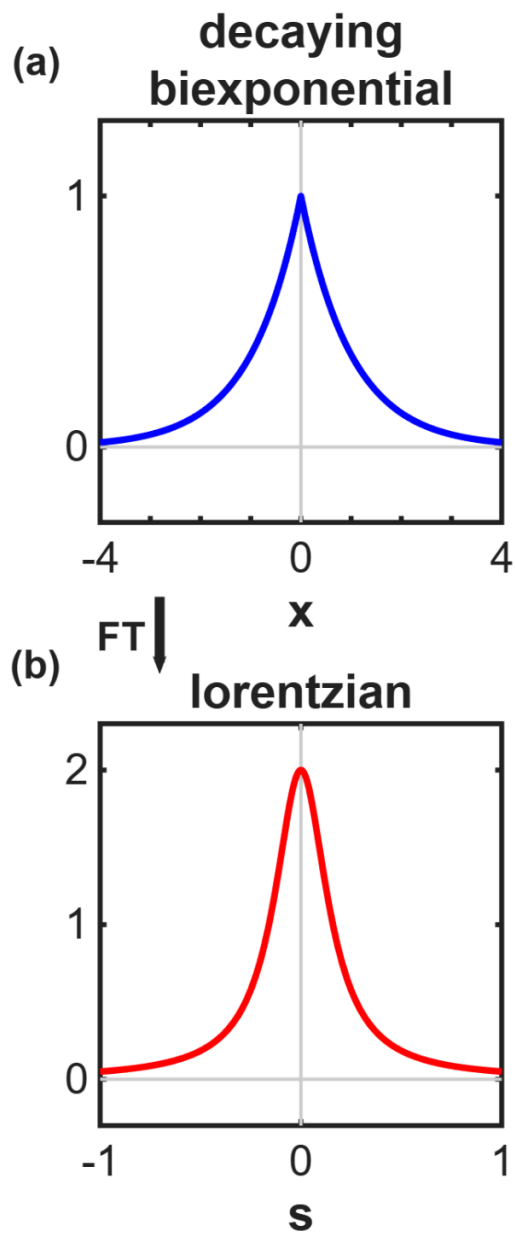


Figure 23. The (a) Decaying biexponential ($e^{-|x|}$), and (b) Lorentzian ($\frac{2}{1+4\pi^2 s^2}$) Fourier transform pair.

10. The Decaying biexponential – Lorentzian pair

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

$$\int_{-\infty}^{\infty} e^{-a|x|} e^{-i2\pi s x} dx \quad (122)$$

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

$$\begin{aligned} \int_{-\infty}^{\infty} e^{-a|x|} e^{-i2\pi s x} dx & \quad (123) \\ &= \int_{-\infty}^0 e^{ax} e^{-i2\pi s x} dx \\ &+ \int_0^{\infty} e^{-ax} e^{-i2\pi s x} dx \\ &= \int_{-\infty}^0 e^{(a-i2\pi s)x} dx + \int_0^{\infty} e^{-(a+i2\pi s)x} dx = \frac{1}{a-i2\pi s} e^{(a-i2\pi s)x} \Big|_{-\infty}^0 \\ &+ \frac{-1}{a+i2\pi s} e^{-(a+i2\pi s)x} \Big|_0^{\infty} = \frac{1}{a-i2\pi s} + \frac{1}{a+i2\pi s} \\ &= \frac{2a}{a^2 + 4\pi^2 s^2} \end{aligned}$$

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 22).

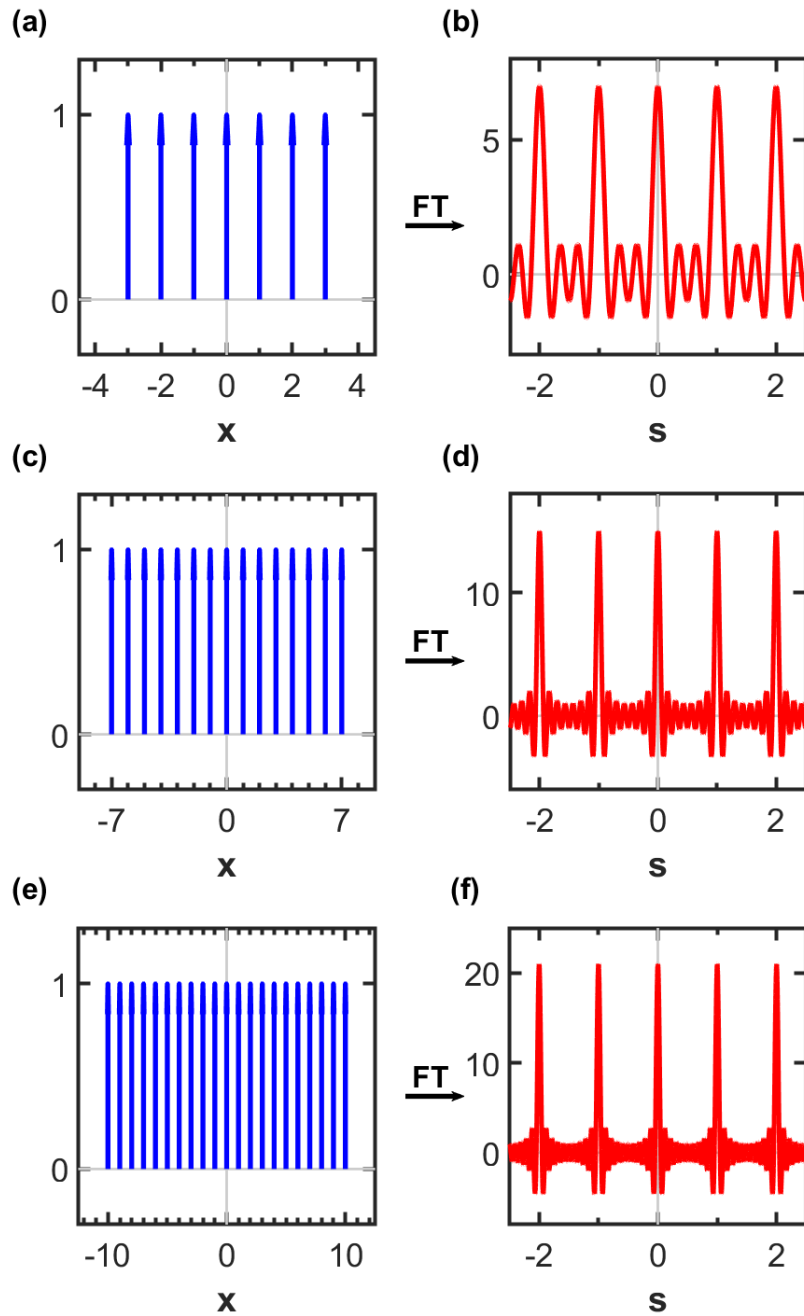


Figure 24. The results of Fourier transforming $\text{III}_m(x)$, i.e., $\mathcal{F}(\text{III}_m(x))$, for (a–b) $m = 3$, (c–d) $m = 7$, (e–f) and $m = 10$, which provides a justification the shah function being its own Fourier transform.

11. Shah-shah pair

It turns out that the shah function is its own Fourier transform. That is $\text{III}(x) \leftrightarrow \text{III}(s)$ (see Figure 24). We published a short tutorial article in Vacuum Technology & Coating that explains why this could be the case.⁴¹ We took Fourier transforms of finite sums of delta function pairs around $x = 0$ (the middle of $\text{III}(x)$) and also the middle delta function of $\text{III}(x)$. That is, we considered Equation 101 over increasing, symmetric limits that were not $-\infty$ and ∞ . For example, Equation 124 shows Equation 101 as a partial sum, $\tilde{\text{III}}_m(x)$, extending from $-m$ to m , where m is an integer, and Figure 24 shows the results of Fourier transforming $\tilde{\text{III}}_m(x)$, i.e., $\mathcal{F}(\tilde{\text{III}}_m(x))$, for $m = 3, 7$, and 10 . As m increases, $\mathcal{F}(\tilde{\text{III}}_m(x))$ increasingly looks like $\text{III}(s)$.

$$\tilde{\text{III}}_m(x) = \sum_{n=-m}^m \delta(x - n) \quad (124)$$

The following argument helps explain why $\mathcal{F}(\tilde{\text{III}}_m(x))$ turns into $\text{III}(s)$ as $m \rightarrow \infty$. First, when $m = 1$, $\tilde{\text{III}}_1(x) = \delta(x) + \delta(x - 1) + \delta(x + 1)$ and $\mathcal{F}(\tilde{\text{III}}_1(x)) = 1 + 2\cos(2\pi s)$, where, in general, $\mathcal{F}(\delta(x - n) + \delta(x + n)) = 2\cos(2\pi ns)$. These results mean that each cosine created by a pair of delta functions at equal distances, n , from the y-axis creates a cosine ($\cos(2\pi ns)$) 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 $\delta(x + 1)$. That is, n is the frequency of the reciprocal space function $\cos(2\pi ns)$. Because n is an integer, $\cos(2\pi ns)$ has a value of unity at all integer values of s , so there is constructive interference of the $\cos(2\pi ns)$ 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 $\mathcal{F}(e^{-\pi(ax)^2} * e^{-\pi(bx)^2})$? We invoke the convolution theorem, which tells us that $\mathcal{F}(e^{-\pi(ax)^2} * e^{-\pi(bx)^2}) = \frac{1}{|a|} e^{-\pi(s/a)^2} \cdot \frac{1}{|b|} e^{-\pi(s/b)^2} = \frac{1}{|ab|} e^{-\pi s^2 (1/a^2 + 1/b^2)}$. We define $1/c^2 = 1/a^2 + 1/b^2$, which gives us $\frac{1}{|ab|} e^{-\pi(s/c)^2}$. Thus, with a little algebra, $\frac{|c|}{|ab|} \mathcal{F}^{-1}\left(\frac{1}{|c|} e^{-\pi(s/c)^2}\right) = \frac{|c|}{|ab|} e^{-\pi(cx)^2} = \frac{|c|}{|ab|} e^{-\pi c^2 x^2}$. That is, $e^{-\pi(ax)^2} * e^{-\pi(bx)^2} = \frac{|c|}{|ab|} e^{-\pi c^2 x^2}$.

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

First, the example in the previous section 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 $c^2 = \frac{a^2 b^2}{a^2 + b^2}$, which allows us to also write $c^2 = \frac{a^2}{(\frac{a}{b})^2 + 1}$ and $c^2 = \frac{b^2}{(\frac{b}{a})^2 + 1}$. However, because $(\frac{a}{b})^2 + 1 > 1$ and $(\frac{b}{a})^2 + 1 > 1$, 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 function that is broader 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. Another exception to this ‘rule’ will be seen in the Hilbert transform below.

Third, when a broad Gaussian is convolved with a narrow Gaussian, we basically just get the broad Gaussian back. To show this, we consider $e^{-\pi(ax)^2} * e^{-\pi(bx)^2} = \frac{|c|}{|ab|} e^{-\pi c^2 x^2}$ 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 $e^{-\pi c^2 x^2} \approx e^{-\pi b^2 x^2}$. Thus, for $a \gg b$, $e^{-\pi(ax)^2} * e^{-\pi(bx)^2} \approx \frac{1}{|a|} e^{-\pi b^2 x^2}$. 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 $\frac{1}{2}(\delta(x+a) + \delta(x-a)) \leftrightarrow \cos(2\pi as)$. Accordingly, $\cos(2\pi at) \leftrightarrow \frac{1}{2}(\delta(f+a) + \delta(f-a))$. 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:

$$\begin{aligned}\mathcal{F}\{f(t)\cos(2\pi at)\} &= F(f) * \frac{1}{2}(\delta(f+a) + \delta(f-a)) \\ &= \frac{1}{2}(F(f+a) + F(f-a))\end{aligned}\tag{125}$$

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.

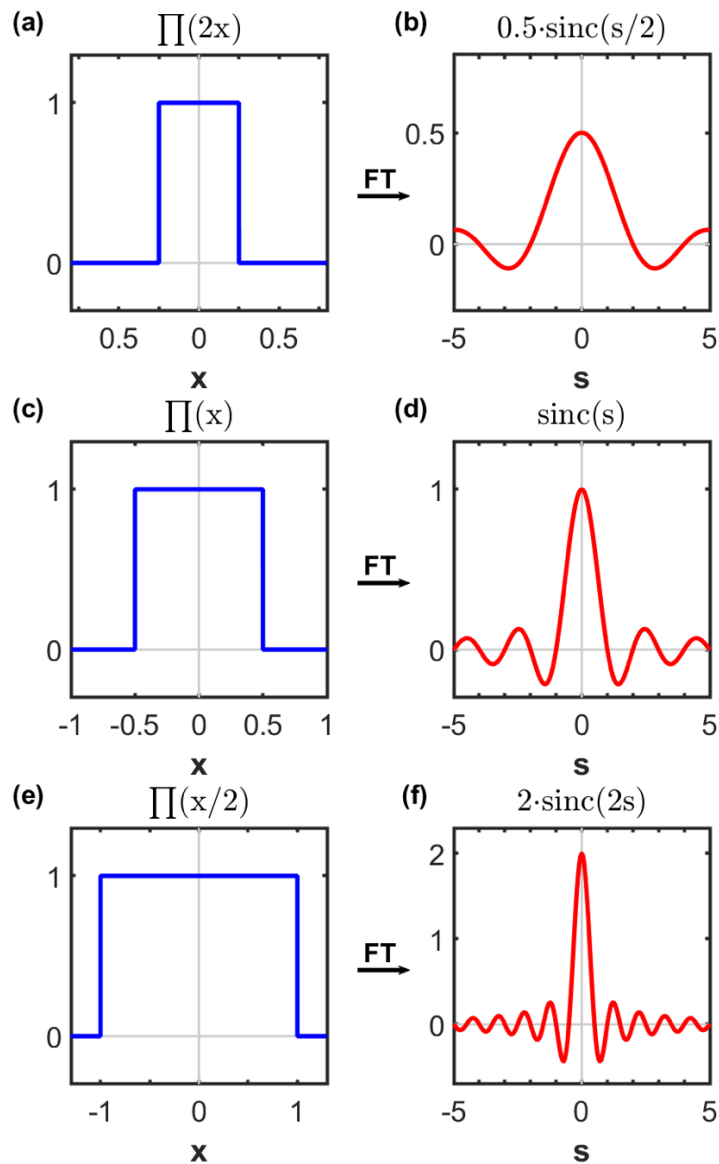


Figure 25. Illustration of the reciprocal nature of three Fourier transforms. (a, c, e), three boxcar functions are becoming progressively broader, while in (b, d, f) their Fourier transforms (sinc functions) are becoming progressively narrower.

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, or functions with sharper features, have broader Fourier transforms, and broad functions without sharp features have narrower Fourier transforms. 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 74), 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 25 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 that extend 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:

$$f(x) = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} f(\tau)e^{-i2\pi s\tau}d\tau \right] e^{i2\pi sx}ds \quad (126)$$

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

$$f(x) = \int_{-\infty}^{\infty} f(\tau) \left[\int_{-\infty}^{\infty} e^{-i2\pi s\tau} e^{i2\pi sx}ds \right] d\tau \quad (127)$$

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 127 is the inverse Fourier transform of $e^{-i2\pi s\tau}$, which means that this inner integral must be $\delta(x - \tau)$. Thus, Equation 127 becomes:

$$f(x) = \int_{-\infty}^{\infty} f(\tau)\delta(x - \tau)d\tau = f(x) \quad (128)$$

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:

$$\mathcal{F}\mathcal{F}f = \mathcal{F}F = \int_{-\infty}^{\infty} F(s)e^{-i2\pi sx}ds = \int_{-\infty}^{\infty} F(s)e^{i2\pi(-x)s}ds = f(-x) \quad (129)$$

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 $\mathcal{F}\mathcal{F}\mathcal{F}\mathcal{F}f = f$ for any function.

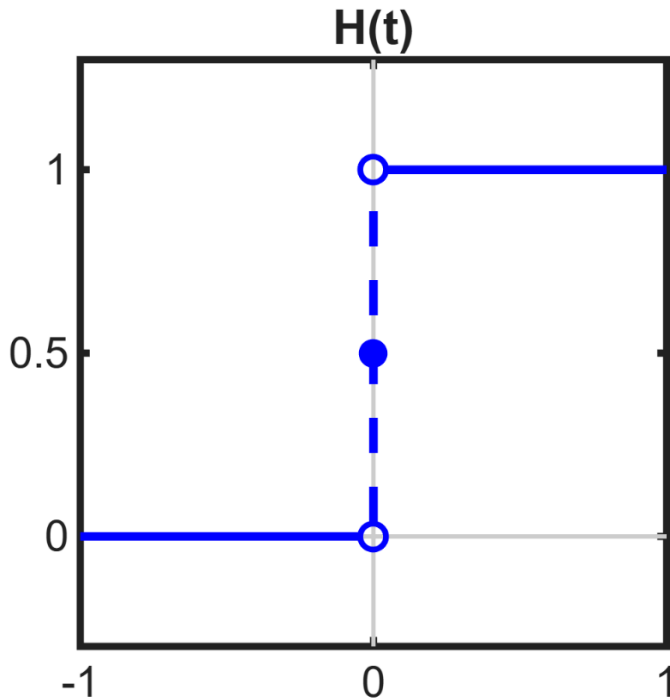


Figure 26. The Heaviside step function, $H(t)$, as defined in Equation 130. In Equation 130, $H(t)$ is not defined at $t = 0$.

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 26), $H(t)$, is named after 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 $t < 0$, unity for $t > 0$, and $\frac{1}{2}$ at $t = 0$. That is:

$$H(t) = \begin{cases} 1 & \text{for } t > 0 \\ \frac{1}{2} & \text{at } t = 0 \\ 0 & \text{for } t < 0 \end{cases} \quad (130)$$

Obviously, $H(t)$ can be defined differently at $t = 0$, where the resulting functions differ from each other by a null function.

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

The Heaviside step function, $H(t)$, can be obtained by integrating across the delta function as follows:

$$H(t) = \int_{-\infty}^t \delta(t') dt' \quad (131)$$

Accordingly, the delta function can be seen as the derivative of the Heaviside step function. This idea is illustrated in Figure 27, where as $a \rightarrow 0$, the function in Figure 27a becomes the Heaviside step function and its derivative (Figure 27b) become a delta function.

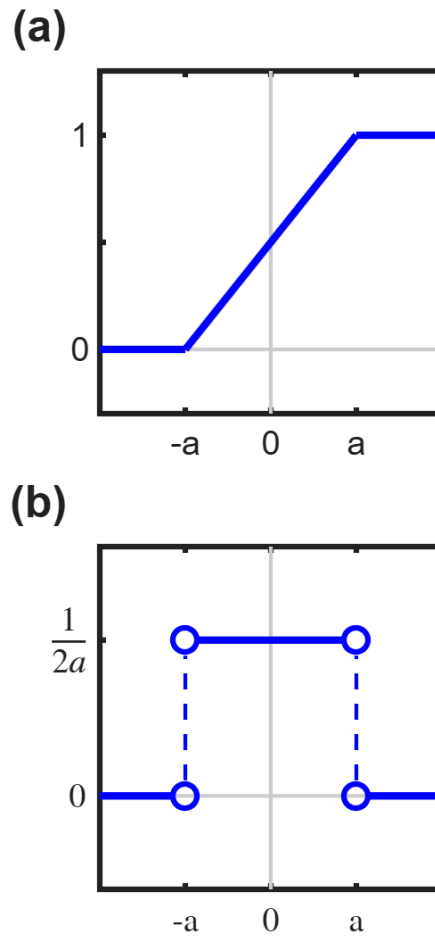


Figure 27. (a) The edge of a function that becomes the Heaviside step function as $a \rightarrow 0$, and (b) the derivative of this function, which becomes a delta function as $a \rightarrow 0$. That is, as $a \rightarrow 0$, the height of the function in (b) goes to infinity and its width goes to zero while the area of the function remains constant at unity.

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:

$$R(x) = \begin{cases} x, & x > 0 \\ 0, & x < 0 \end{cases} \quad (132)$$

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

$$R(x) = \int_{-\infty}^x H(x') dx' \quad (133)$$

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

The top hat function may be defined via $H(x)$ as follows:

$$\Pi(x) = H\left(x + \frac{1}{2}\right) + H\left(-x + \frac{1}{2}\right) - 1 \quad (134)$$

Because we can now differentiate the Heaviside step function, we can discuss the following example, which reveals some nice internal consistency within Fourier theory. Figure 28a shows a top hat function, $2 \cdot \Pi(x)$, which, again, can be viewed as made up of two Heaviside step functions (Equation 134), and Figure 28b shows its Fourier transform $2 \cdot \text{sinc}(s)$. Figure 28c then shows the derivative of $2 \cdot \Pi(x)$, which is $2 \cdot \left(\delta\left(x + \frac{1}{2}\right) - \delta\left(x - \frac{1}{2}\right)\right)$, and Figure 28d shows the Fourier transform of $2 \cdot \left(\delta\left(x + \frac{1}{2}\right) - \delta\left(x - \frac{1}{2}\right)\right)$, which is $4i \cdot \sin(\pi s)$. The internal consistency here is that we can use the derivative theorem to obtain the result in Figure 28d directly from the top hat function in Figure 28a. That is, $\frac{d}{dx}(2 \cdot \Pi(x)) \leftrightarrow i2\pi s \cdot 2 \frac{\sin(\pi s)}{\pi s} = 4i \cdot \sin(\pi s)$.

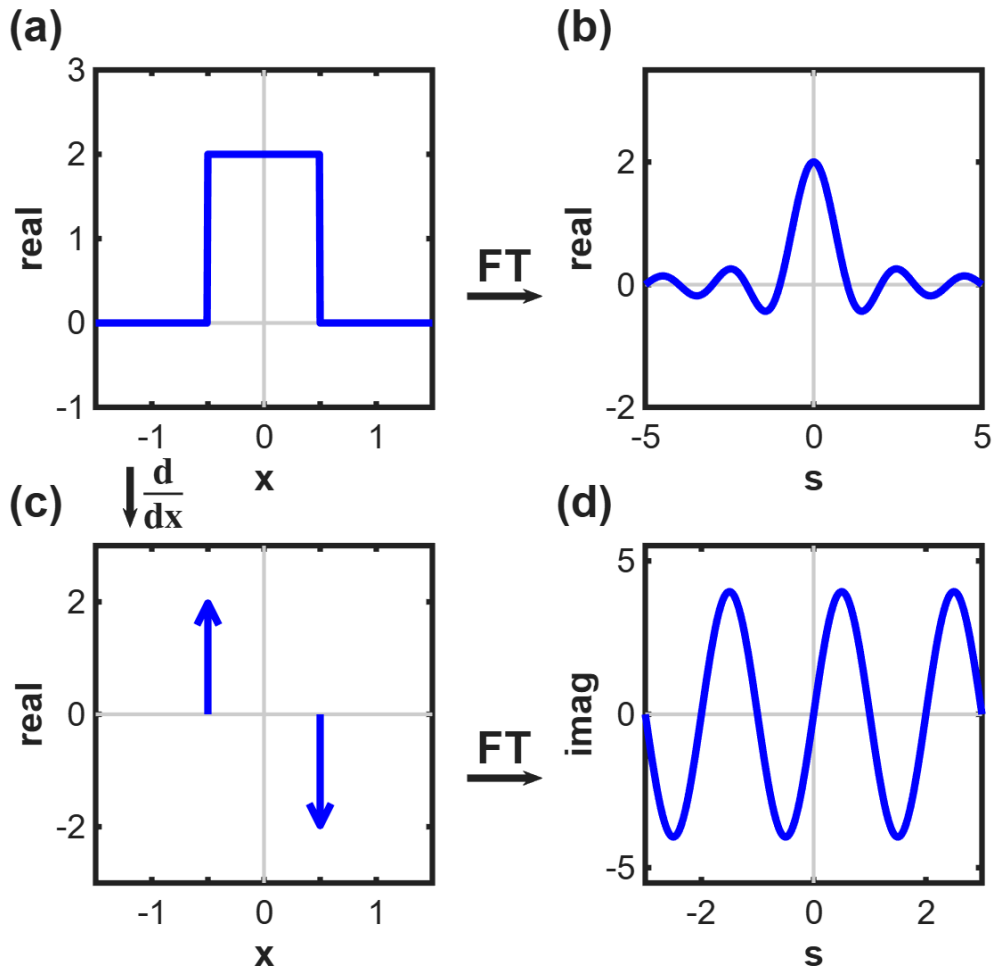


Figure 28. (a) A top hat function, $2 \cdot \Pi(x)$, and (b) its Fourier transform $2 \cdot \text{sinc}(s)$. (c) The derivative of $2 \cdot \Pi(x)$, which is $2 \cdot \left(\delta\left(x + \frac{1}{2}\right) - \delta\left(x - \frac{1}{2}\right) \right)$, and (d) its Fourier transform $4i \cdot \sin(\pi s)$.

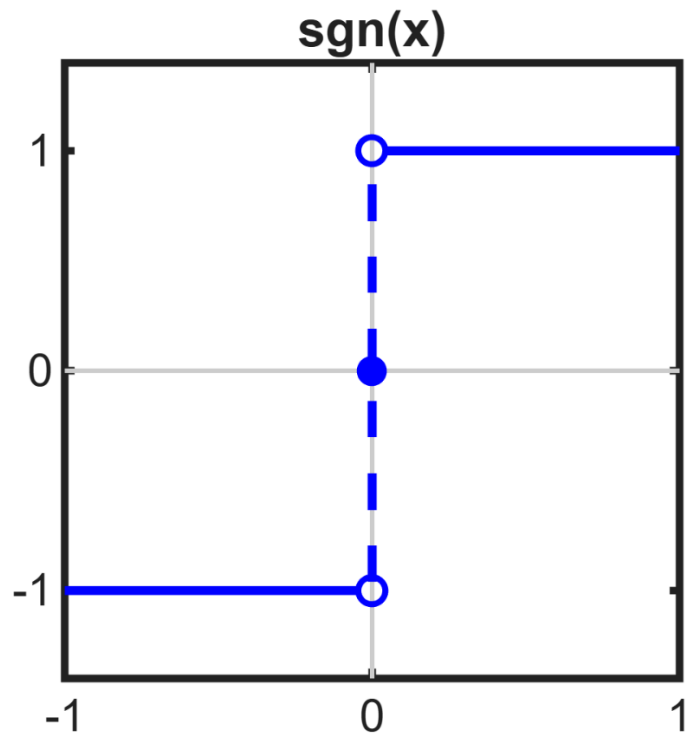


Figure 29. The signum, or sign function, $\text{sgn}(x)$, as defined in Equation 135.

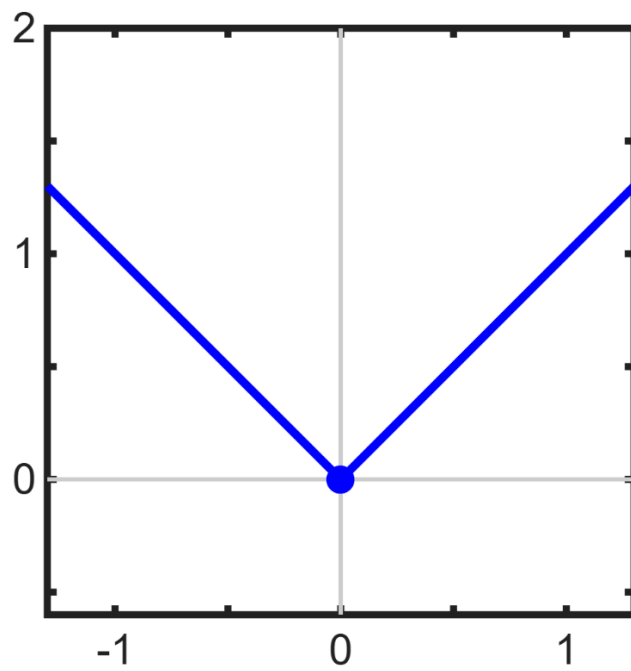


Figure 30. The function $x \cdot \text{sgn}(x)$.

2. The signum or sign function

The signum, or sign, function (see Figure 29), $\text{sgn}(x)$, is defined as:

$$\text{sgn}(x) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{at } x = 0 \\ -1 & \text{for } x < 0 \end{cases} \quad (135)$$

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: $\text{sgn}(x) = 2H(x) - 1$.

As an example of its use, \ Figure 30 shows $x \text{sgn}(x)$, 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 $\Lambda'(x) = -\Pi\left(\frac{x}{2}\right) \text{sgn}(x)$, where $\Lambda'(x)$ is the derivative of the triangle function. This can be shown by rewriting $\Lambda(x)$ as:

$$\Lambda(x) = \begin{cases} 1 - x, & 0 < x < 1 \\ 1 + x, & -1 < x < 0 \\ 0, & |x| > 1 \end{cases} \quad (136)$$

Thus:

$$\Lambda'(x) = \begin{cases} -1, & 0 < x < 1 \\ 1, & -1 < x < 0 \\ 0, & |x| > 1 \end{cases} \quad (137)$$

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

$$\Pi\left(\frac{x}{2}\right) = \begin{cases} 1, & -1 < x < 0 \\ 1, & 0 < x < 1 \\ 0, & |x| > 1 \end{cases} \quad (138)$$

Accordingly:

$$-\Pi\left(\frac{x}{2}\right) = \begin{cases} -1, & -1 < x < 0 \\ -1, & 0 < x < 1 \\ 0, & |x| > 1 \end{cases} \quad (139)$$

And finally:

$$-\Pi\left(\frac{x}{2}\right) \operatorname{sgn}(x) = \begin{cases} 1, & -1 < x < 0 \\ -1, & 0 < x < 1 \\ 0, & |x| > 1 \end{cases} \quad (140)$$

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

3. *The Fourier transform of the signum function, $\operatorname{sgn}(x)$*

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

$$\lim_{a \rightarrow \infty} e^{\frac{-1}{a}|x|} \operatorname{sgn}(x) \quad (141)$$

We now consider the Fourier transform of this function, which will consist of breaking it into two integrals, combining terms, performing the integrations, and considering the limit as $a \rightarrow \infty$:

$$\lim_{a \rightarrow \infty} \int_{-\infty}^{\infty} e^{\frac{-1}{a}|x|} \operatorname{sgn}(x) e^{-i2\pi s x} dx \quad (142)$$

$$\begin{aligned} &= -\lim_{a \rightarrow \infty} \int_{-\infty}^0 e^{\frac{1}{a}x} e^{-i2\pi s x} dx + \lim_{a \rightarrow \infty} \int_0^{\infty} e^{\frac{-1}{a}x} e^{-i2\pi s x} dx \\ &= -\lim_{a \rightarrow \infty} \int_{-\infty}^0 e^{\left(\frac{1}{a} - i2\pi s\right)x} dx \\ &\quad + \lim_{a \rightarrow \infty} \int_0^{\infty} e^{\left(-\frac{1}{a} - i2\pi s\right)x} dx \\ &= \lim_{a \rightarrow \infty} \left(\frac{-1}{\frac{1}{a} - i2\pi s} e^{\left(\frac{1}{a} - i2\pi s\right)x} \Big|_{-\infty}^0 \right) \\ &\quad + \lim_{a \rightarrow \infty} \left(\frac{1}{-\frac{1}{a} - i2\pi s} e^{\left(-\frac{1}{a} - i2\pi s\right)x} \Big|_0^{\infty} \right) = \lim_{a \rightarrow \infty} \frac{-1}{\frac{1}{a} - i2\pi s} \\ &\quad - \lim_{a \rightarrow \infty} \frac{1}{-\frac{1}{a} - i2\pi s} = \frac{-1}{-i2\pi s} + \frac{-1}{-i2\pi s} = \frac{1}{i\pi s} \end{aligned}$$

This proof may seem like cheating, but it is not. The $e^{\left(\frac{1}{a} - i2\pi s\right)x}$ term can be rewritten as $e^{\left(\frac{x}{a}\right)} e^{-i2\pi s x}$, 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 $e^{\left(\frac{-\infty}{\infty}\right)}$. However, 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, $\mathcal{F}(\text{sgn}(x)) = \frac{1}{i\pi s}$, we can easily obtain the Fourier transform of the Heaviside step function, where $H(x) = \frac{1}{2}(\text{sgn}(x) + 1)$. Thus:

$$\mathcal{F}(H(x)) = \mathcal{F}\left(\frac{1}{2}(\text{sgn}(x) + 1)\right) = \mathcal{F}\left(\frac{1}{2}\text{sgn}(x)\right) + \mathcal{F}\left(\frac{1}{2}\right) = \frac{1}{2i\pi s} + \frac{1}{2}\delta(s) \quad (143)$$

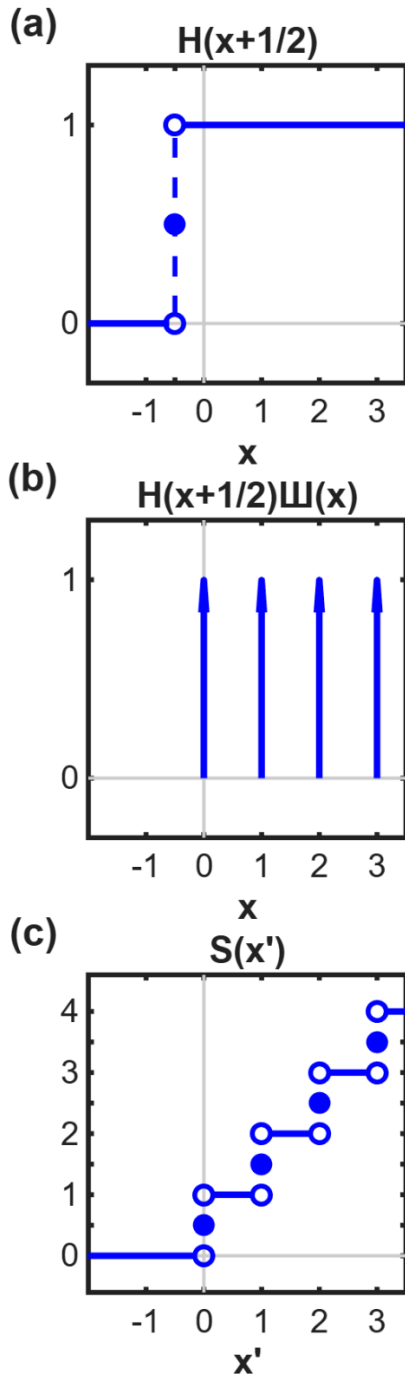


Figure 31. (a) The function $H\left(x + \frac{1}{2}\right)$, which is a shifted Heaviside step function, (b) The function $H\left(x + \frac{1}{2}\right)\text{III}(x)$, and (c) The integral $S(x') = \int_{-\infty}^{x'} H\left(x + \frac{1}{2}\right)\text{III}(x)dx$ for different values of x' . Note: the delta functions that the $\text{III}(x)$ 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 $H\left(x + \frac{1}{2}\right) \mathbb{I}\mathbb{I}(x)$ and $S(x')$, which are the integrand and function in Equation 144 (see answer/plots in Figure 31).

$$S(x') = \int_{-\infty}^{x'} H\left(x + \frac{1}{2}\right) \mathbb{I}\mathbb{I}(x) dx \quad (144)$$

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

A while ago, the students in a Linford group meeting were 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 $\tau > 0$:

$$\lim_{\tau \rightarrow 0} \int_{-\infty}^{\infty} -x\tau^{-2} \Pi\left(\frac{x}{2\tau}\right) \text{sgn}(x) dx = -1 \quad (145)$$

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:

$$\lim_{\tau \rightarrow 0} \tau^{-2} \int_{-\tau}^{\tau} -x \operatorname{sgn}(x) dx \quad (146)$$

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

$$2 \lim_{\tau \rightarrow 0} \tau^{-2} \int_0^{\tau} -x \operatorname{sgn}(x) dx \quad (147)$$

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

$$2 \lim_{\tau \rightarrow 0} \tau^{-2} \int_0^{\tau} -x dx \quad (148)$$

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

$$-2 \lim_{\tau \rightarrow 0} \tau^{-2} \frac{\tau^2}{2} \quad (149)$$

Thus, τ and 2 cancel out of the equation, the $\lim_{\tau \rightarrow 0}$ term turns out to be unnecessary, and we are left with the desired result of -1 .

O. Another way of writing the inverse Fourier transform

We are now familiar with the inverse Fourier transform: $f(x) = \int_{-\infty}^{\infty} F(s)e^{i2\pi sx} ds$. Another way to write this inverse, which comes in handy when the Fast Fourier Transform is formulated, is using complex conjugates, as follows:

$$f(x) = \left[\int_{-\infty}^{\infty} F^*(s)e^{-i2\pi sx} ds \right]^* \quad (150)$$

The advantage here is that now both the (forward) Fourier transform and inverse Fourier transform involve the same kernel ($e^{-i2\pi sx}$). We can show that Equation 150 is equivalent to our original definition of the inverse Fourier transform by expanding $F(s)$ into its real and imaginary parts, $F(s) = F_{real}(s) + iF_{imag}(s)$, in Equation 150, as follows:

$$\begin{aligned}
& \left[\int_{-\infty}^{\infty} F^*(s) e^{-i2\pi s x} ds \right]^* \tag{151} \\
&= \left[\int_{-\infty}^{\infty} (F_{real}(s) - iF_{imag}(s)) (\cos(2\pi s x) - i \sin(2\pi s x)) ds \right]^* \\
&= \left[\int_{-\infty}^{\infty} F_{real}(s) \cos(2\pi s x) - F_{imag}(s) \sin(2\pi s x) \right. \\
&\quad \left. - iF_{real}(s) \sin(2\pi s x) - iF_{imag}(s) \cos(2\pi s x) ds \right]^* \\
&= \int_{-\infty}^{\infty} F_{real}(s) \cos(2\pi s x) - F_{imag}(s) \sin(2\pi s x) \\
&\quad + iF_{real}(s) \sin(2\pi s x) + iF_{imag}(s) \cos(2\pi s x) ds \\
&= \int_{-\infty}^{\infty} F_{real}(s) (\cos(2\pi s x) + i \sin(2\pi s x)) \\
&\quad + iF_{imag}(s) (\cos(2\pi s x) + i \sin(2\pi s x)) ds = \\
&= \int_{-\infty}^{\infty} F_{real}(s) e^{i2\pi s x} + iF_{imag}(s) e^{i2\pi s x} ds = \int_{-\infty}^{\infty} F(s) e^{i2\pi s x}
\end{aligned}$$

P. *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, not continuous, so Equation 6 ($F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi sx} dx$) cannot be used as naturally with them. Later in this article, we discuss the discrete Fourier transform, which provides a way to calculate the Fourier transforms of discrete data. First, however, we'll extend the Fourier transform to multiple dimensions and discuss the Hilbert transform.

VI. The Two-Dimensional Fourier transform and the Fourier transform in higher dimensions

The Fourier transform can be extended to higher dimensions. Commenting on moving beyond of a single dimension in Fourier analysis, Bracewell observed: “In two dimensions phenomena are richer...”²² In this section, we prove some of the theorems associated with the two-dimensional Fourier transform. In general, these proofs use the same logic as their one-dimensional analogs. We will also explore some of the ‘richer phenomena’ Bracewell alluded to.

A. *The two-dimensional Fourier transform*

The two-dimensional Fourier transform of a function of two variables, $f(x, y)$, can be written as:

$$F(s, r) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) e^{-i2\pi(sx+ry)} dx dy \quad (152)$$

or

$$F(s, r) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) (\cos(2\pi(sx + ry)) - i \sin(2\pi(sx + ry))) dx dy \quad (153)$$

and the inverse Fourier transform of $F(s, r)$ is:

$$f(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(s, r) e^{i2\pi(sx + ry)} ds dr \quad (154)$$

or

$$f(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(s, r) (\cos(2\pi(sx + ry)) + i \sin(2\pi(sx + ry))) ds dr \quad (155)$$

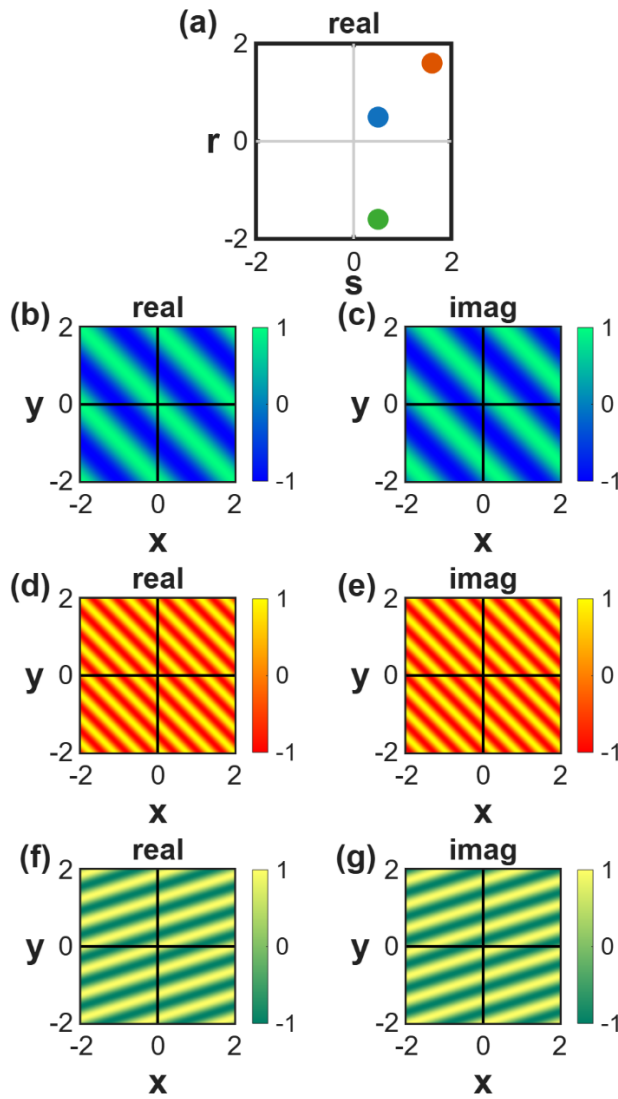


Figure 32. Real and imaginary parts of a few of the many waves that a function is multiplied by to generate a 2D Fourier transform. (a) Three selected values of s and r . (b - c) The real and imaginary waves corresponding to the blue point in (a). (d - e) The real and imaginary waves corresponding to the red point in (a). (f - g) The real and imaginary waves corresponding to the green point in (a).

B. Examples of the kernel of the 2D Fourier transform

To help the reader better understand the 2D Fourier transform, Figure 32 shows the kernel of the 2D Fourier transform ($e^{i2\pi(sx+ry)}$) plotted for three values of s and r . These sinusoids are a few of the waves that a function, $f(x, y)$, is multiplied by to create a 2D Fourier transform, $F(s, r)$. Notice in Figure 32 that points in s/r space that are closer to the origin produce lower frequency waves, and vice versa.

C. *Extension of the 2D Fourier transform to even higher dimensions*

Note the $sx + ry$ terms in Equations 152 and 154. If we consider (s, r) and (x, y) to be real-valued vectors, then their dot product is $sx + ry$. Thus, if we define $\mathbf{s} = (s, r)$ and $\mathbf{x} = (x, y)$ we can rewrite Equations 152 and 154 as:

$$F(\mathbf{s}) = \int_{-\infty}^{\infty} f(\mathbf{x}) e^{-i2\pi(\mathbf{s} \cdot \mathbf{x})} d\mathbf{x} \quad (156)$$

$$f(\mathbf{x}) = \int_{-\infty}^{\infty} F(\mathbf{s}) e^{i2\pi(\mathbf{s} \cdot \mathbf{x})} d\mathbf{s} \quad (157)$$

where $d\mathbf{x}$ and $d\mathbf{s}$ imply double integrals over $dx dy$ and $ds dr$, respectively.

It may appear that Equations 156 and 157 have done nothing except, perhaps, make Equations 152 and 154 more abstract. However, what we now have provides a natural extension of the Fourier transform to higher dimensions. That is, if $\mathbf{s} = (s_1, s_2, s_3, \dots, s_m)$ and $\mathbf{x} =$

$(x_1, x_2, x_3, \dots, x_m)$, we can use Equations 156 and 157 to define the Fourier transform in m dimensions, where $d\mathbf{x}$ and $d\mathbf{s}$ now imply integration over all m variables/dimensions. One can also write Equations 156 and 157 as $F(\mathbf{s}) = \int_{\mathbb{R}^m} f(\mathbf{x}) e^{-i2\pi(\mathbf{s} \cdot \mathbf{x})} d\mathbf{x}$ and $f(\mathbf{x}) = \int_{\mathbb{R}^m} F(\mathbf{s}) e^{i2\pi(\mathbf{s} \cdot \mathbf{x})} d\mathbf{s}$.

D. Separability of the 2D-Fourier transform (and the Fourier transform in higher dimensions)

If $f(x, y)$ in Equation 152 is separable, i.e., if $f(x, y) = g(x)h(y)$, and if $g(x) \leftrightarrow G(s)$ and $h(y) \leftrightarrow H(r)$, we can rewrite Equation 152 as:

$$\begin{aligned}
 F(s, r) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) e^{-i2\pi(sx+ry)} dx dy \\
 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x)h(y) e^{-i2\pi(sx+ry)} dx dy \\
 &= \int_{-\infty}^{\infty} g(x) e^{-i2\pi sx} dx \int_{-\infty}^{\infty} h(y) e^{-i2\pi ry} dy = G(s)H(r)
 \end{aligned} \tag{158}$$

Following the logic in Equation 158, this derivation can be extended to higher dimensions. That is, for $\mathbf{s} = (s_1, s_2, s_3, \dots, s_m)$ and $\mathbf{x} = (x_1, x_2, x_3, \dots, x_m)$, i.e., m dimensions, and if $f(\mathbf{x}) = \prod_{k=1}^m f_k(x_k)$ and $f_k(x_k) \leftrightarrow F_k(s_k)$, for $k = 1 \dots m$, the m -dimensional Fourier transform of $f(\mathbf{x})$ is $\prod_{k=1}^m F_k(s_k)$. Function separability simplifies Fourier analysis in higher dimensions.

E. The delta function in higher dimensions

The delta function can be defined in multiple dimensions. For example, the delta function in two dimensions, ${}^2\delta(x, y)$, is defined as:

$${}^2\delta(x, y) = \delta(x)\delta(y) \quad (159)$$

The integral of ${}^2\delta(x, y)$ can be shown to be unity as follows:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} {}^2\delta(x, y) \, dx dy = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(x)\delta(y) \, dx dy = \int_{-\infty}^{\infty} \delta(x) \, dx \int_{-\infty}^{\infty} \delta(y) \, dy = 1 \quad (160)$$

Note that the integral $\int_{-\infty}^{\infty} \delta(x) \, dx$ implies that the units of $\delta(x)$ are $1/\text{length}$, and the integral $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(x)\delta(y) \, dx dy$ implies that the units of ${}^2\delta(x, y)$ are $1/\text{area}$.

The delta function is similarly defined in three dimensions as ${}^3\delta(x, y, z) = \delta(x)\delta(y)\delta(z)$, where:

$$\begin{aligned} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} {}^3\delta(x, y, z) \, dx dy dz & \quad (161) \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(x)\delta(y)\delta(z) \, dx dy dz \\ &= \int_{-\infty}^{\infty} \delta(x) \, dx \int_{-\infty}^{\infty} \delta(y) \, dy \int_{-\infty}^{\infty} \delta(z) \, dz = 1 \end{aligned}$$

This function, ${}^3\delta(x,y,z)$, might represent a point mass at the origin, where its units are $1/volume$.

The delta function can be defined similarly in higher dimensions.

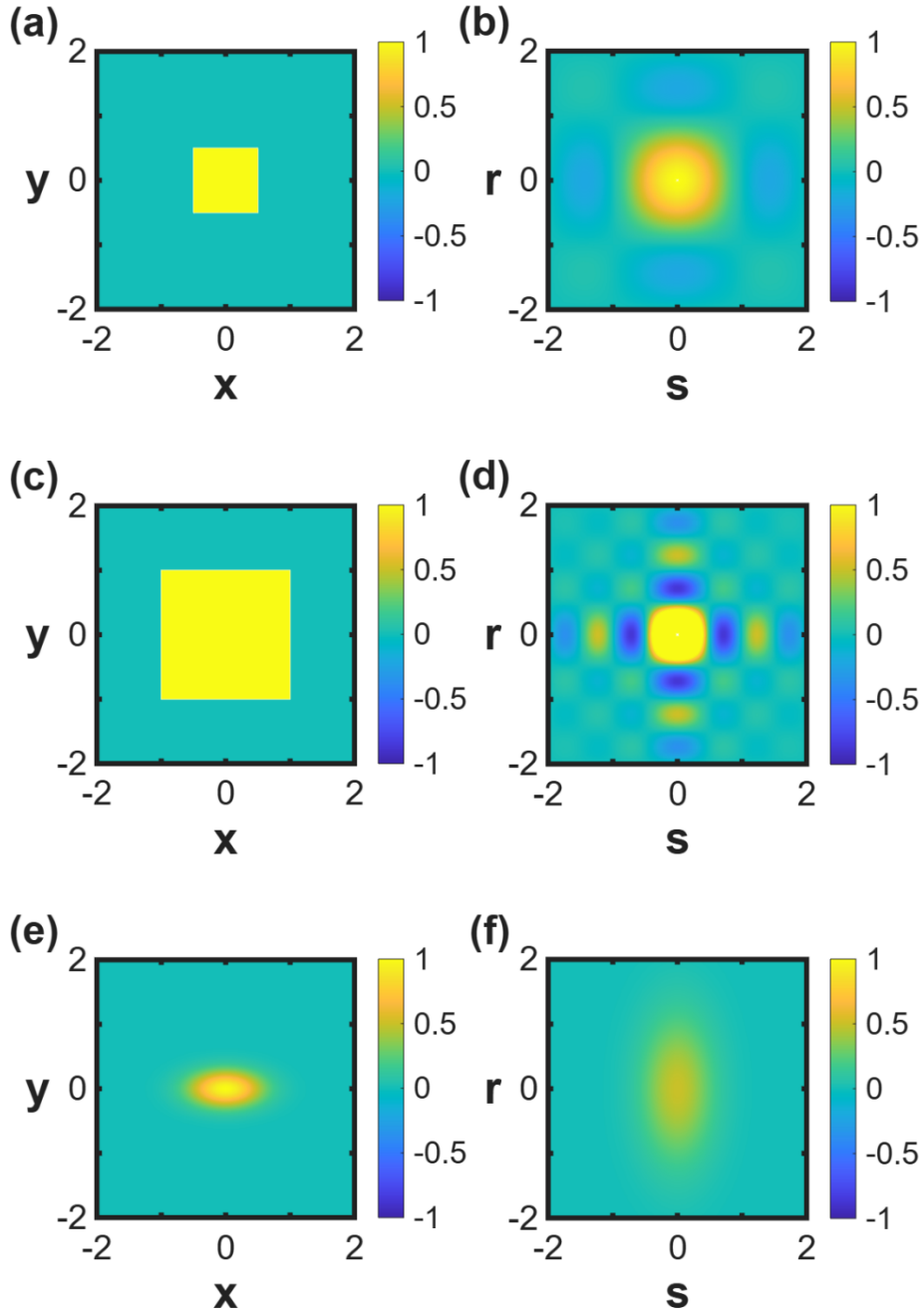


Figure 33. (a) Separable two-dimensional function: $\Pi(x)\Pi(y)$ and (b) its two-dimensional Fourier transform: $\text{sinc}(s)\text{sinc}(r)$. (c) Separable two-dimensional function: $\Pi\left(\frac{x}{2}\right)\Pi\left(\frac{y}{2}\right)$ and (d) its two-dimensional Fourier transform: $4 \cdot \text{sinc}(2s)\text{sinc}(2r)$. (e) Separable two-dimensional function: $e^{-\pi x^2} e^{-\pi(2y)^2}$ and (f) its two-dimensional Fourier transform: $e^{-\pi s^2} \frac{1}{2} e^{-\pi\left(\frac{r}{2}\right)^2}$.

F. Examples of the 2D Fourier transforms of separable functions

Example 1. Figure 33a shows the two-dimensional separable function: $\Pi(x)\Pi(y)$, which is the product of two boxcar functions. Because this function is separable, its two-dimensional Fourier transform is: $\text{sinc}(s)\text{sinc}(r)$ (see Figure 33b), where $\Pi(x) \leftrightarrow \text{sinc}(s)$ and $\Pi(y) \leftrightarrow \text{sinc}(r)$. (Note that Equations 11 and 13 give the definitions of the boxcar function, $\Pi(x)$, and $\text{sinc}(x)$ functions, respectively.) Furthermore, Figure 33c and Figure 33d show the two-dimensional plot of $\Pi\left(\frac{x}{2}\right)\Pi\left(\frac{y}{2}\right)$ and its Fourier transform $4\text{sinc}(2s)\text{sinc}(2r)$, respectively, which highlight the separability of this function and the reciprocal relationship between functions and their transforms in Fourier analysis.

Example 2. From $e^{-\pi x^2} \leftrightarrow e^{-\pi s^2}$ and $e^{-\pi(2x)^2} \leftrightarrow \frac{1}{2}e^{-\pi\left(\frac{s}{2}\right)^2}$ we have $e^{-\pi x^2}e^{-\pi(2y)^2} \leftrightarrow e^{-\pi s^2}\frac{1}{2}e^{-\pi\left(\frac{r}{2}\right)^2}$ (see Figure 33e – f), where we are also using the double-headed arrow to indicate the 2D Fourier transform.

G. Theorems and definitions for the two-dimensional Fourier transform

1. The linearity theorem

If $f(x, y) \leftrightarrow F(s, r)$ and $g(x, y) \leftrightarrow G(s, r)$ what is the two-dimensional Fourier transform of $a \cdot f(x, y) + b \cdot g(x, y)$, where a and b are constants? Inserting $a \cdot f(x, y) + b \cdot g(x, y)$ into the formula for the two-dimensional Fourier transform gives

$$\begin{aligned}
& \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (a \cdot f(x, y) + b \cdot g(x, y)) e^{-i2\pi(sx+ry)} dx dy & (162) \\
&= a \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) e^{-i2\pi(sx+ry)} dx dy \\
&+ b \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x, y) e^{-i2\pi(sx+ry)} dx dy = a \cdot F(s, r) + b \cdot G(s, r)
\end{aligned}$$

That is, $a \cdot f(x, y) + b \cdot g(x, y) \leftrightarrow a \cdot F(s, r) + b \cdot G(s, r)$.

The logic behind this theorem may seem a little repetitive and perhaps even somewhat tedious at this point (and below). Nevertheless, we *have* just derived an important result that should not be overlooked. If we need to take the Fourier transform of a function, and we find that this function is the sum of two functions that have known Fourier transforms, we can easily obtain the Fourier transform of our function via this theorem. Of course, it follows that, for m functions $f_i(x, y)$ with Fourier transforms $F_i(s, r)$ and constants c_i : $\sum_{i=1}^m c_i \cdot f_i(x, y) \leftrightarrow \sum_{i=1}^m c_i \cdot F_i(s, r)$.

2. *The inversion theorem*

In this section, we ask the question. If $f(x, y) \leftrightarrow F(s, r)$, what is the Fourier transform of $F(x, y)$? That is, what is:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(x, y) e^{-i2\pi(sx+ry)} dx dy \quad (163)$$

We rewrite this slightly as:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(x, y) e^{i2\pi((-s)x + (-r)y)} dx dy \quad (164)$$

That is, Equation 164 allows us to see this problem as an inverse Fourier transform. Thus:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(x, y) e^{i2\pi((-s)x + (-r)y)} dx dy = f(-s, -r) \quad (165)$$

so $F(x, y) \leftrightarrow f(-s, -r)$.

3. *The shift theorem in two dimensions*

Consider a two-dimensional function and its Fourier transform: $f(x, y) \leftrightarrow F(s, r)$. Now imagine that $f(x, y)$ has been shifted by amounts a and b , which are real numbers, to produce the shifted function $f(x - a, y - b)$. What is the two-dimensional Fourier transform of $f(x - a, y - b)$?

We write:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x - a, y - b) e^{-i2\pi(sx + ry)} dx dy \quad (166)$$

We now make the change of variables: $x' = x - a$ and $y' = y - b$, which leads to:

$$\begin{aligned}
& \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x', y') e^{-i2\pi(s(x'+a)+r(y'+b))} dx' dy' & (167) \\
&= e^{-i2\pi(sa+rb)} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x', y') e^{-i2\pi(sx'+ry')} dx' dy' \\
&= e^{-i2\pi(sa+rb)} F(s, r)
\end{aligned}$$

Thus, $f(x - a, y - b) \leftrightarrow e^{-i2\pi(sa+rb)} F(s, r)$.

4. Definition of convolution in two dimensions

For two functions of two variables, $f(x, y)$ and $g(x, y)$, we can indicate their two-dimensional convolution, $h(x, y)$, as $h(x, y) = f(x, y) ** g(x, y)$, which we can define mathematically as:

$$h(x, y) = f(x, y) ** g(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\tau, \sigma) g(x - \tau, y - \sigma) d\tau d\sigma \quad (168)$$

As in the one-dimensional case, in a two-dimensional convolution, we still have one function, $f(\tau, \sigma)$, that remains the same in the integral (unshifted and not reversed), while the other function, $g(x - \tau, y - \sigma)$, is reversed in both variables and shifted to every possible position with respect to the first one.

5. The convolution theorem in two dimensions

We now derive the convolution theorem in two dimensions. To do this, we consider the two-dimensional Fourier transform of $h(x, y) = f(x, y) ** g(x, y)$, where $f(x, y) \leftrightarrow F(s, r)$, $g(x, y) \leftrightarrow G(s, r)$, and $h(x, y) \leftrightarrow H(s, r)$, as follows:

$$\begin{aligned}
 H(s, r) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [f(x, y) ** g(x, y)] e^{-i2\pi(sx+ry)} dx dy \\
 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\tau, \sigma) g(x - \tau, y - \sigma) d\tau d\sigma \right] e^{-i2\pi(sx+ry)} dx dy
 \end{aligned} \tag{169}$$

We change the order of integration:

$$H(s, r) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\tau, \sigma) \left[\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x - \tau, y - \sigma) e^{-i2\pi(sx+ry)} dx dy \right] d\tau d\sigma \tag{170}$$

and apply the shift theorem in two dimensions ($f(x - a, y - b) \leftrightarrow e^{-i2\pi(sa+rb)} F(s, r)$), which gives:

$$\begin{aligned}
H(s, r) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\tau, \sigma) [e^{-i2\pi(s\tau+r\sigma)} G(s, r)] d\tau d\sigma \\
&= G(s, r) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\tau, \sigma) e^{-i2\pi(s\tau+r\sigma)} d\tau d\sigma = F(s, r)G(s, r)
\end{aligned} \tag{171}$$

Thus, $h(x, y) = f(x, y) ** g(x, y) \leftrightarrow H(s, r) = F(s, r)G(s, r)$, so, as was the case in one dimension, we again have the very important result that convolution in one domain is equivalent to multiplication in the reciprocal domain. This result is used heavily in image processing.

6. *The derivative theorem in two dimensions*

To derive the derivative theorem, we begin with Equation 154, taking the partial derivatives of both sides of this equation with respect to x and y , as follows:

$$\begin{aligned}
\frac{\partial}{\partial x} \frac{\partial}{\partial y} f(x, y) &= \frac{\partial}{\partial x} \frac{\partial}{\partial y} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(s, r) e^{i2\pi(sx+ry)} ds dr & (172) \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\partial}{\partial x} \frac{\partial}{\partial y} (F(s, r) e^{i2\pi(sx+ry)}) ds dr \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\frac{\partial}{\partial x} e^{i2\pi s x} \right) \left(\frac{\partial}{\partial y} e^{i2\pi r y} \right) F(s, r) ds dr \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (i2\pi s) e^{i2\pi s x} (i2\pi r) e^{i2\pi r y} F(s, r) ds dr \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (i2\pi s)(i2\pi r) F(s, r) e^{i2\pi(sx+ry)} ds dr =
\end{aligned}$$

Thus, $\frac{\partial}{\partial x} \frac{\partial}{\partial y} f(x, y) \leftrightarrow (i2\pi s)(i2\pi r)F(s, r)$.

Note that repeating this process gives $\frac{\partial^m}{\partial x^m} \frac{\partial^n}{\partial y^n} f(x, y) \leftrightarrow (i2\pi s)^m (i2\pi r)^n F(s, r)$.

VII. The Hilbert transform. A transform in direct space that is best calculated via Fourier analysis

The Fourier transform shows up all over advanced mathematics and signal processing. As an example of this, we consider the Hilbert transform. The Hilbert transform is an unusual example of a repeated convolution that does not broaden a function.

The Hilbert transform of a function, $f(x)$, is defined as:

$$h(x) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{x - \tau} f(\tau) d\tau \quad (173)$$

Note that this definition constitutes a convolution, i.e., $h(x) = \frac{1}{\pi x} * f(x)$. Consequently, the Hilbert transform of a function does not create a function in another domain, e.g., reciprocal space, as the Fourier transform does. Rather the Hilbert transform transforms a function in direct space into another function in direct space.

Note that the number of figures and their detail in this section may be a little more than is necessary to explain the Hilbert transform. Ultimately, however, we decided to leave them in because of the tutorial nature of this document.

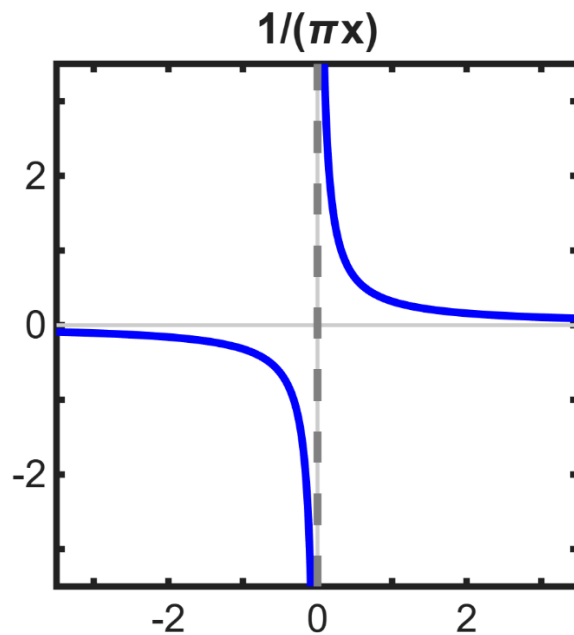


Figure 34. The kernel of the Hilbert transform: $\frac{1}{\pi x}$.

Unfortunately, the integral (the convolution) in Equation 173 can be challenging to deal with because of the $\frac{1}{x-\tau}$ term in it, which has a singularity. For example, Figure 34 shows the kernel of the Hilbert transform: $\frac{1}{\pi x}$, which has a singularity at zero. Of course, because it is a convolution, the Hilbert transform can also be written as:

$$h(x) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{\tau} f(x - \tau) d\tau \quad (174)$$

As we noted in a previous article,^{42, 43} if the math in Equation 173 is performed directly, it must be done with principal values (P.V.) because permitting the two limits for the two branches of the Hilbert transform integral to be different, as shown in Equation 175, can lead to mathematical absurdities. Also, in Equation 175, we have also used a script, capital $\mathcal{H}$ to indicate a Hilbert transform.

$$\begin{aligned} \mathcal{H}(f(x))(x) &= h(x) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f(\tau)}{x - \tau} d\tau \\ &= \frac{1}{\pi} \left(\lim_{\varepsilon_1 \rightarrow 0} \int_{-\infty}^{x-\varepsilon_1} \frac{f(\tau)}{x - \tau} d\tau + \lim_{\varepsilon_2 \rightarrow 0} \int_{x+\varepsilon_2}^{\infty} \frac{f(\tau)}{x - \tau} d\tau \right) \end{aligned} \quad (175)$$

Accordingly, we write correctly:

$$\mathcal{H}(f(x))(x) = h(x) = \frac{1}{\pi} P.V. \int_{-\infty}^{\infty} \frac{f(\tau)}{x - \tau} d\tau \quad (176)$$

$$= \frac{1}{\pi} \left(\lim_{\varepsilon \rightarrow 0} \int_{-\frac{1}{\varepsilon}}^{x-\varepsilon} \frac{f(\tau)}{x - \tau} d\tau + \int_{x+\varepsilon}^{\frac{1}{\varepsilon}} \frac{f(\tau)}{x - \tau} d\tau \right)$$

which keeps the limits the same.

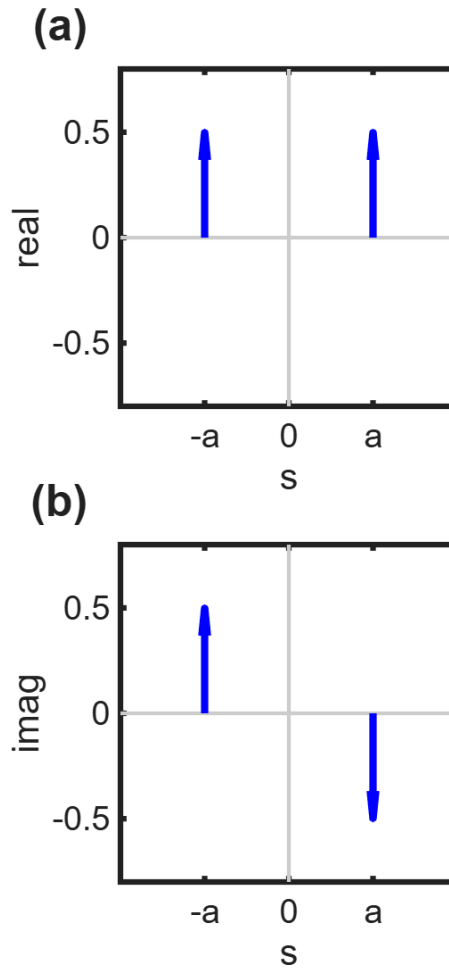


Figure 35. The Fourier transforms of (a) $\cos(2\pi ax)$, which is $\frac{1}{2}(\delta(s+a) + \delta(s-a))$, and (b) $\sin(2\pi ax)$, which is $i \cdot \frac{1}{2}(\delta(s+a) - \delta(s-a))$. Notice that the y-axes in these plots are different, i.e., real and imaginary.

Most commonly, the Hilbert transform is obtained via Fourier analysis and the convolution theorem. Using the convolution theorem, where we are assuming that $f(x) \leftrightarrow F(s)$, we find that $\mathcal{F}\{h(x)\}(x) = \mathcal{F}\left\{\frac{1}{\pi x} * f(x)\right\}(x) = \mathcal{F}\left\{\frac{1}{\pi x}\right\} \cdot F(s)$ or $h(x) = \mathcal{F}^{-1}\left\{\mathcal{F}\left\{\frac{1}{\pi x}\right\} \cdot F(s)\right\}$. Now, it turns out that $\mathcal{F}\left\{\frac{1}{\pi x}\right\} = -i \cdot \text{signum}(s)$. This is a very important result. In other words, $h(x) = \mathcal{F}^{-1}\{-i \cdot \text{signum}(s) \cdot F(s)\}$.

We now explore the Hilbert transform using $h(x) = \mathcal{F}^{-1}\{-i \cdot \text{signum}(s) \cdot F(s)\}$ for the cosine and sine functions. We have learned that $\cos(2\pi ax) \leftrightarrow \frac{1}{2}(\delta(s+a) + \delta(s-a))$ and $\sin(2\pi ax) \leftrightarrow i \cdot \frac{1}{2}(\delta(s+a) - \delta(s-a))$, where these Fourier transforms (pairs of delta functions) are (again) shown in Figure 35.

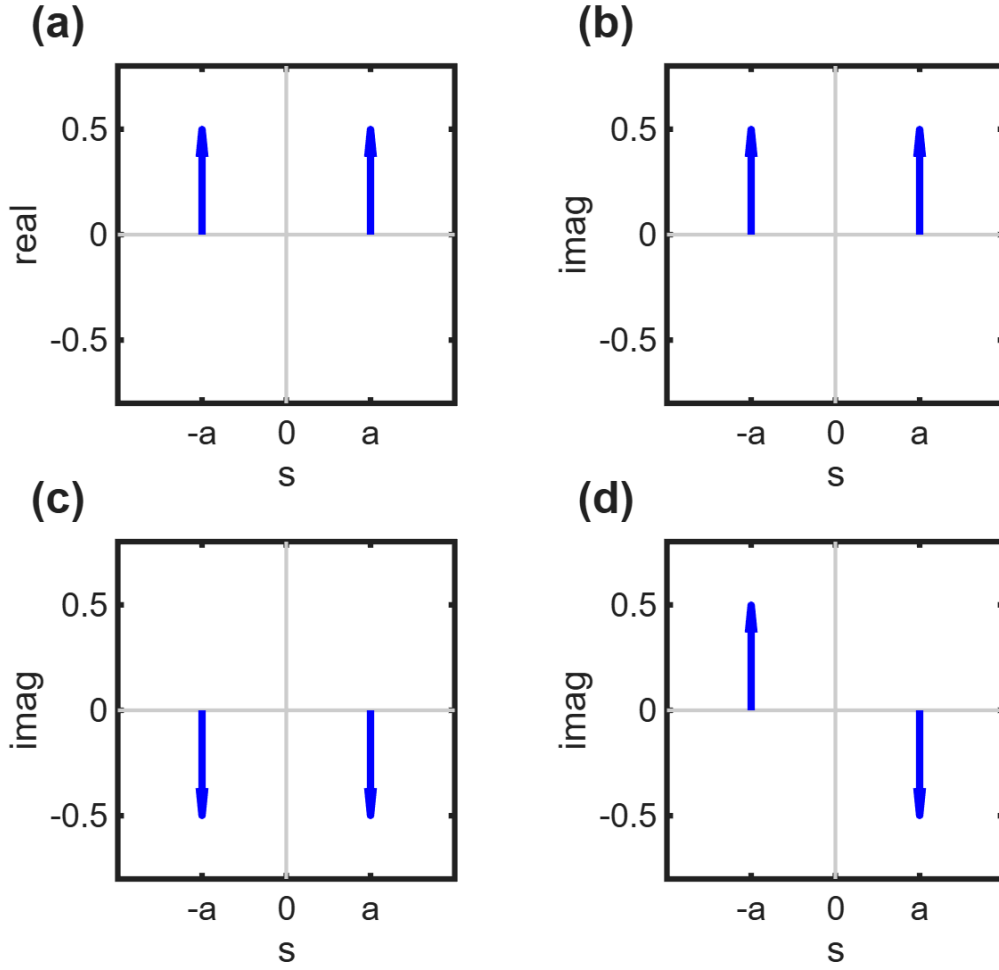


Figure 36. The process of going from $\frac{1}{2}(\delta(s+a) + \delta(s-a))$, which is the Fourier transform of $\cos(2\pi ax)$, to $-i \cdot \text{signum}(s) \cdot \frac{1}{2}(\delta(s+a) + \delta(s-a))$, which is the Fourier transform of the Hilbert transform of $\cos(2\pi ax)$. That is, (a) shows $\frac{1}{2}(\delta(s+a) + \delta(s-a))$, (b) shows $i \cdot \frac{1}{2}(\delta(s+a) + \delta(s-a))$, i.e., the delta functions in (a) have been rotated 90° in complex space, (c) shows $-i \cdot \frac{1}{2}(\delta(s+a) + \delta(s-a))$, and finally (d) shows $-i \cdot \text{signum}(s) \cdot \frac{1}{2}(\delta(s+a) + \delta(s-a))$.

Now, the Hilbert transform of $\cos(2\pi ax)$ is $\mathcal{F}^{-1}\left\{-i \cdot \text{signum}(s) \cdot \frac{1}{2}(\delta(s+a) + \delta(s-a))\right\}$. Figure 36 shows the process of going from $\frac{1}{2}(\delta(s+a) + \delta(s-a))$ to $-i \cdot \text{signum}(s) \cdot \frac{1}{2}(\delta(s+a) + \delta(s-a))$ in reciprocal space. That is, Figure 36a shows $\frac{1}{2}(\delta(s+a) + \delta(s-a))$, Figure 36b shows $i \cdot \frac{1}{2}(\delta(s+a) + \delta(s-a))$, where the delta functions have been

rotated $+90^\circ$ into the complex plane, Figure 36c shows $-i \frac{1}{2}(\delta(s+a) + \delta(s-a))$, which flips them 180° in the complex plane, and Figure 36d shows $-i \cdot \text{signum}(s) \cdot \frac{1}{2}(\delta(s+a) + \delta(s-a)) = i \cdot \frac{1}{2}(\delta(s+a) - \delta(s-a))$. However, $\sin(2\pi ax) \leftrightarrow i \cdot \frac{1}{2}(\delta(s+a) - \delta(s-a))$, which is the same thing. Thus, the Hilbert transform of $\cos(2\pi ax)$ is $\sin(2\pi ax)$. Importantly, the net effect of the Hilbert transform in Figure 36 is to rotate the original delta functions on the left and right in the figure by 90° and -90° , respectively.

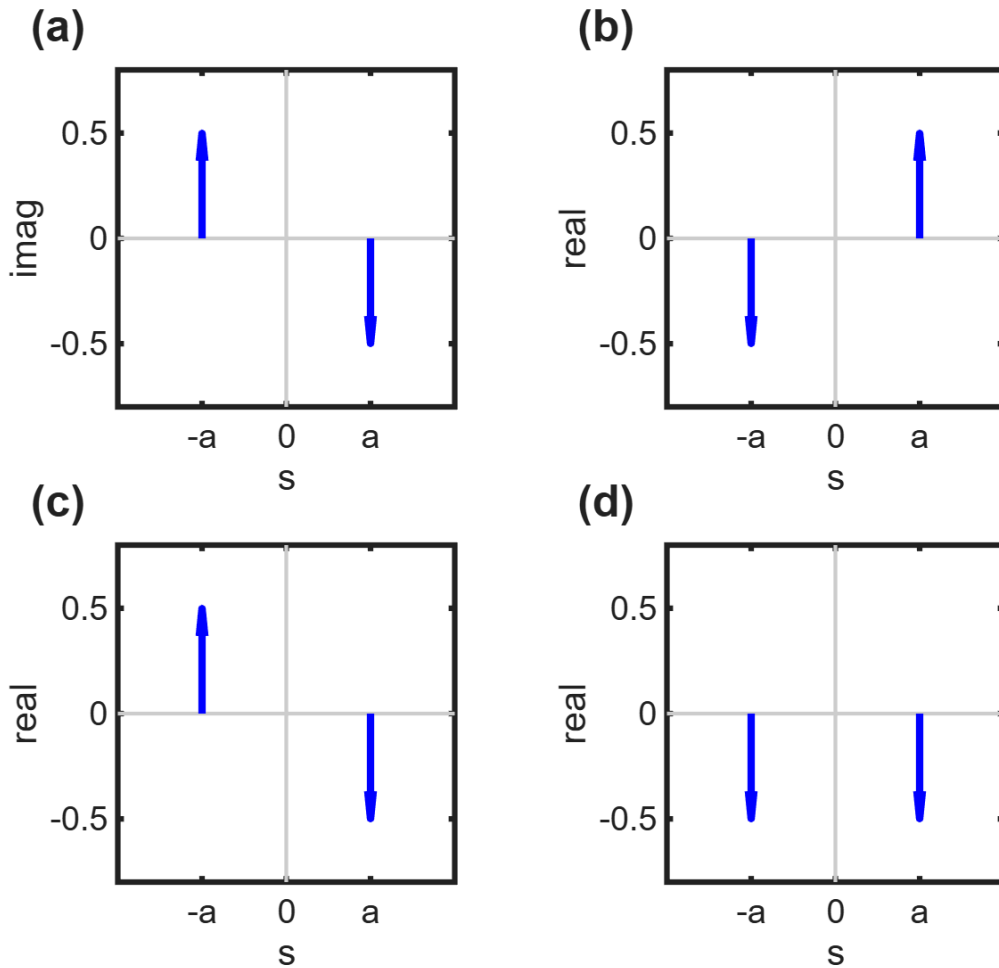


Figure 37. The process of going from $\frac{i}{2}(\delta(s+a) - \delta(s-a))$, which is the Fourier transform of $\sin(2\pi ax)$, to $-i \cdot \text{signum}(s) \cdot \frac{i}{2}(\delta(s+a) - \delta(s-a))$, which is the Fourier transform of the Hilbert transform of $\sin(2\pi ax)$ and also the

Fourier transform of $-\cos(2\pi ax)$. (a) shows $\frac{i}{2}(\delta(s+a) - \delta(s-a))$, (b) shows $i \cdot \frac{i}{2}(\delta(s+a) - \delta(s-a)) = -\frac{1}{2}(\delta(s+a) - \delta(s-a))$, i.e., the delta functions in (a) have been rotated 90° in complex space, (c) shows $-1 \cdot \frac{-1}{2}(\delta(s+a) - \delta(s-a))$, and finally (d) shows $-i \cdot \text{signum}(s) \cdot \frac{i}{2}(\delta(s+a) - \delta(s-a))$.

For $\mathcal{H}(\sin(2\pi ax))(x)$, we again work in reciprocal space. Figure 37a shows $\frac{i}{2}(\delta(s+a) - \delta(s-a))$, which is the Fourier transform of $\sin(2\pi ax)$, which is where we ended up in Figure 36d. Figure 37b shows $\frac{i}{2}(\delta(s+a) - \delta(s-a))$ multiplied by i , Figure 37c shows $\frac{i}{2}(\delta(s+a) - \delta(s-a))$ multiplied by $-i$, and Figure 37d shows $\frac{i}{2}(\delta(s+a) - \delta(s-a))$ multiplied by $-i \cdot \text{signum}(s)$. The function displayed in Figure 37d is the Fourier transform of $-\cos(x)$, so $\mathcal{H}(\sin(2\pi ax))(x) = -\cos(x)$. Again, notice that going from Figure 37a, which is the Fourier transform of $\sin(2\pi ax)$, to the Fourier transform of its Hilbert transform in Figure 37d, the net effect has been to rotate the original delta functions on the left and right in the figure by 90° and -90° , respectively.

We now take the Hilbert transform of $-\cos(2\pi ax)$, where the Fourier transform of $-\cos(2\pi ax)$ is shown in Figure 37d and in Figure 38a. That is, Figure 38 again shows the process of multiplying the Fourier transform of $-\cos(2\pi ax)$ by $-i \cdot \text{signum}(s)$. This process yields the delta functions in Figure 38d, which are the Fourier transform of $-\sin(2\pi ax)$. Thus, the Hilbert transform of $-\cos(2\pi ax)$ is $-\sin(2\pi ax)$. Again, the net effect here has been to rotate the original delta functions on the left and right in Figure 38 by 90° and -90° , respectively.

Finally, in Figure 39, we take the Hilbert transform of $-\sin(2\pi ax)$, where the Fourier transform of $-\sin(2\pi ax)$ is shown in Figure 38d and Figure 39a. As shown in Figure 39, the Hilbert transform of $-\sin(2\pi ax)$ is $\cos(2\pi ax)$, which is where we started. Again, the net effect here has been to rotate the original delta functions on the left and right in Figure 39 by 90° and

-90° , respectively. We have literally come full circle. As a summary, Figure 40 shows the repeated application of the Hilbert transform in reciprocal space starting with the Fourier transform of $\cos(2\pi ax)$.

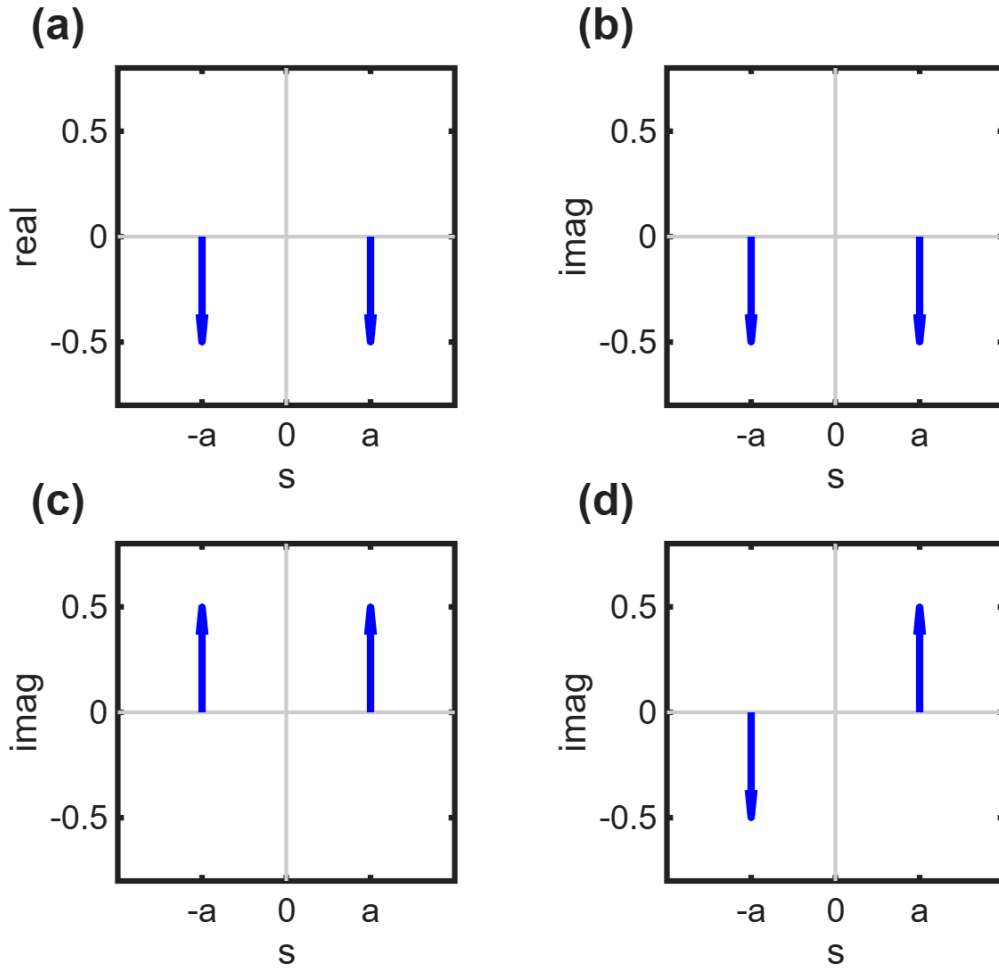


Figure 38. The process of going from $-\frac{1}{2}(\delta(s+a) + \delta(s-a))$, which is the Fourier transform of $-\cos(2\pi ax)$, to $i \cdot \text{signum}(s) \cdot \frac{1}{2}(\delta(s+a) + \delta(s-a))$, which is the Fourier transform of the Hilbert transform of $-\cos(2\pi ax)$. That is, (a) shows $-\frac{1}{2}(\delta(s+a) + \delta(s-a))$, (b) shows $-\frac{i}{2}(\delta(s+a) + \delta(s-a))$, i.e., the delta functions in (a) have been rotated 90° in complex space, (c) shows $\frac{i}{2}(\delta(s+a) + \delta(s-a))$, and finally (d) shows $-i \cdot \text{signum}(s) \cdot \frac{1}{2}(\delta(s+a) + \delta(s-a))$.

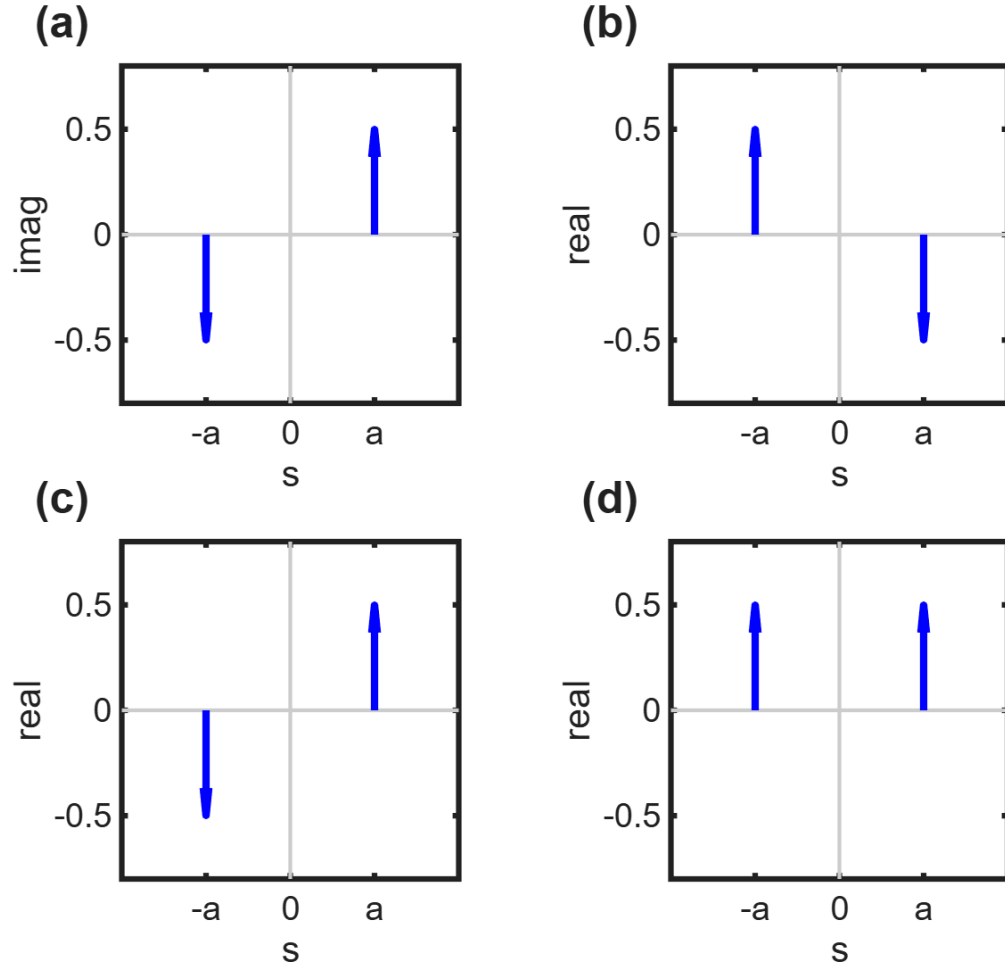


Figure 39. The process of going from $-\frac{i}{2}(\delta(s+a) - \delta(s-a))$, which is the Fourier transform of $-\sin(2\pi ax)$, to $-i \cdot \text{signum}(s) \cdot -\frac{i}{2}(\delta(s+a) - \delta(s-a))$, which is the Fourier transform of the Hilbert transform of $-\sin(2\pi ax)$ and also the Fourier transform of $\cos(2\pi ax)$. (a) shows $-\frac{i}{2}(\delta(s+a) - \delta(s-a))$, (b) shows $i \cdot -\frac{i}{2}(\delta(s+a) - \delta(s-a)) = \frac{1}{2}(\delta(s+a) - \delta(s-a))$, i.e., the delta functions in (a) have been rotated 90° in complex space, (c) shows $-1 \cdot \frac{1}{2}(\delta(s+a) - \delta(s-a))$, and finally (d) shows $-i \cdot \text{signum}(s) \cdot -\frac{i}{2}(\delta(s+a) - \delta(s-a))$.

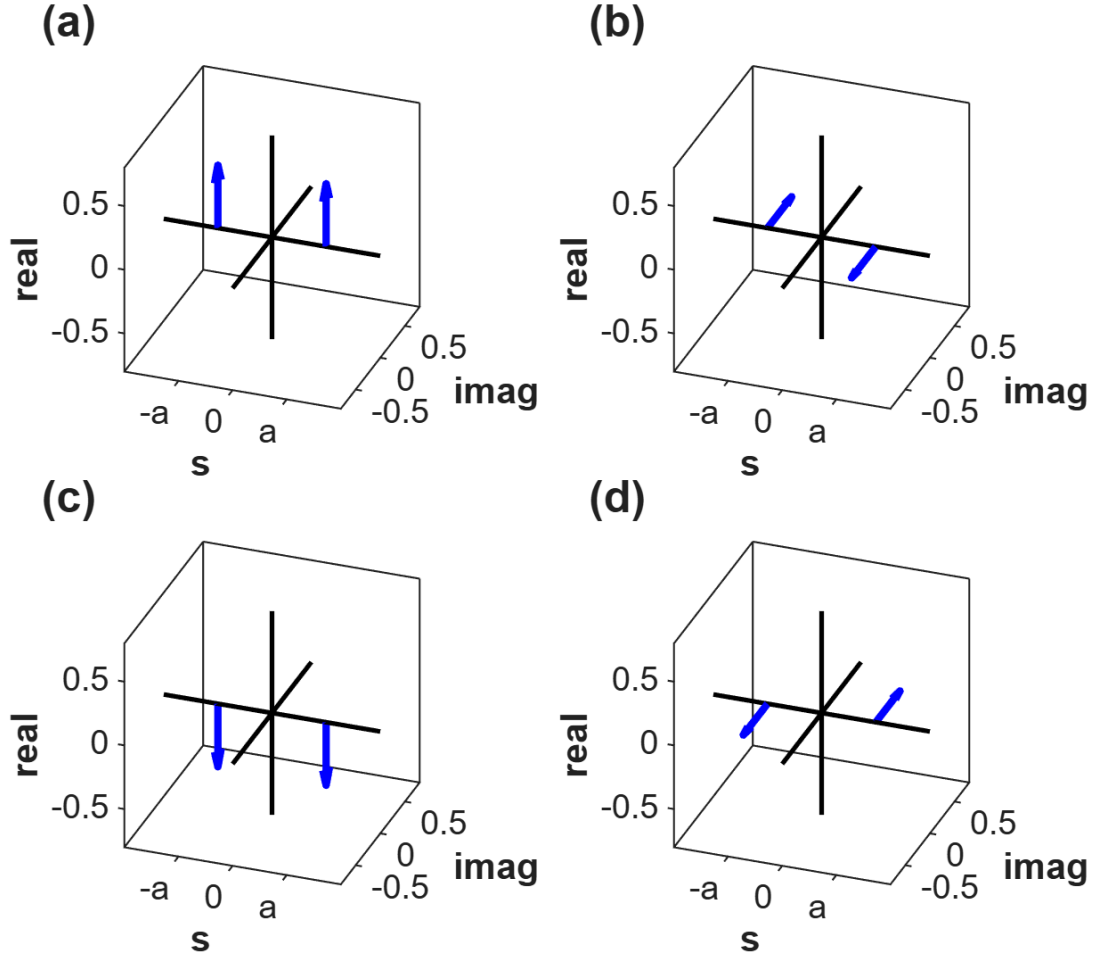


Figure 40. (a) The Fourier transform of $\cos(2\pi ax)$. (b – d) The repeated application of the Hilbert transform to the Fourier transform of $\cos(2\pi ax)$. If the Hilbert transform is applied again to the inverse Fourier transform of the function in (d), $\cos(2\pi ax)$ will again be obtained.

A powerful way to view the Hilbert transform, $h(x) = \mathcal{F}^{-1}\{-i \cdot \text{signum}(s) \cdot F(s)\}$, is in polar coordinates. Again, $f(x)$ is the function to be Hilbert transformed, and $F(s)$ is its Fourier transform. We are assuming here that $F(s)$ can be complex. First, we represent $F(s)$ in terms of its magnitude, $|F(s)|$, and phase, $\theta(s)$: $|F(s)|e^{i\theta(s)}$. Then, step-by-step, we represent $-i \cdot \text{signum}(s)$ in polar coordinates. Multiplication by i is equivalent to multiplication by $e^{\frac{i\pi}{2}}$ (a $+90^\circ$ rotation), and multiplication by $-i$ is equivalent to multiplication by $e^{-\frac{i\pi}{2}}$ (a -90° rotation). Thus,

multiplication by $-i \cdot \text{signum}(s)$ is equivalent to multiplication by $e^{-\frac{i\pi}{2}}$ for $s > 0$ and $e^{\frac{i\pi}{2}}$ for $s < 0$. Thus, for an arbitrary function, $f(x)$, with $f(x) \leftrightarrow F(s)$, $h(x) = \mathcal{F}^{-1} \left\{ e^{-\frac{i\pi}{2}} \cdot |F(s)| e^{i\theta(s)} \right\} = \mathcal{F}^{-1} \left\{ |F(s)| e^{i\theta(s) - \frac{i\pi}{2}} \right\}$ for $s > 0$ and $h(x) = \mathcal{F}^{-1} \left\{ e^{\frac{i\pi}{2}} \cdot |F(s)| e^{i\theta(s)} \right\} = \mathcal{F}^{-1} \left\{ |F(s)| e^{i\theta(s) + \frac{i\pi}{2}} \right\}$ for $s < 0$. The Hilbert transform does not change the magnitude of $F(s)$. Rather, it rotates its phase by either $+90^\circ$ (for $s < 0$) or -90° (for $s > 0$).

As additional examples, Figure 40 and Figure 42 show the creations in reciprocal space of the Hilbert transforms of a Gaussian (the Fourier transform of a Gaussian is another Gaussian) and a biexponentially decaying function (the Fourier transform of this function is a Lorentzian), respectively. To be consist with the other figures in this document, these figures show the process of obtaining these Hilbert transforms in reciprocal space. At this point however, the reader may simply want to verify that the Hilbert transforms in Figure 40d and Figure 42d are the result of rotating the Fourier transforms of the functions in Figure 40a and Figure 42a by $+90^\circ$ or $e^{\frac{i\pi}{2}}$ for $s < 0$ and -90° or $e^{-\frac{i\pi}{2}}$ for $s > 0$. Also, Figure 43 and Figure 44 show the repeated application of the Hilbert transform in reciprocal space to a Gaussian and a biexponentially decaying function. An additional application of the Hilbert transform, which is not shown, would produce the functions in Figure 43a and Figure 44a.

Finally, Figure 45 shows the results in reciprocal space of Hilbert transforming the function: $f(x) = 0$ for $x < 0$ and $f(x) = e^{-x}$ for $x > 0$ three times. This figure is particularly illustrative because $f(x)$ is neither even nor odd and therefore has a Hermitian Fourier transform.

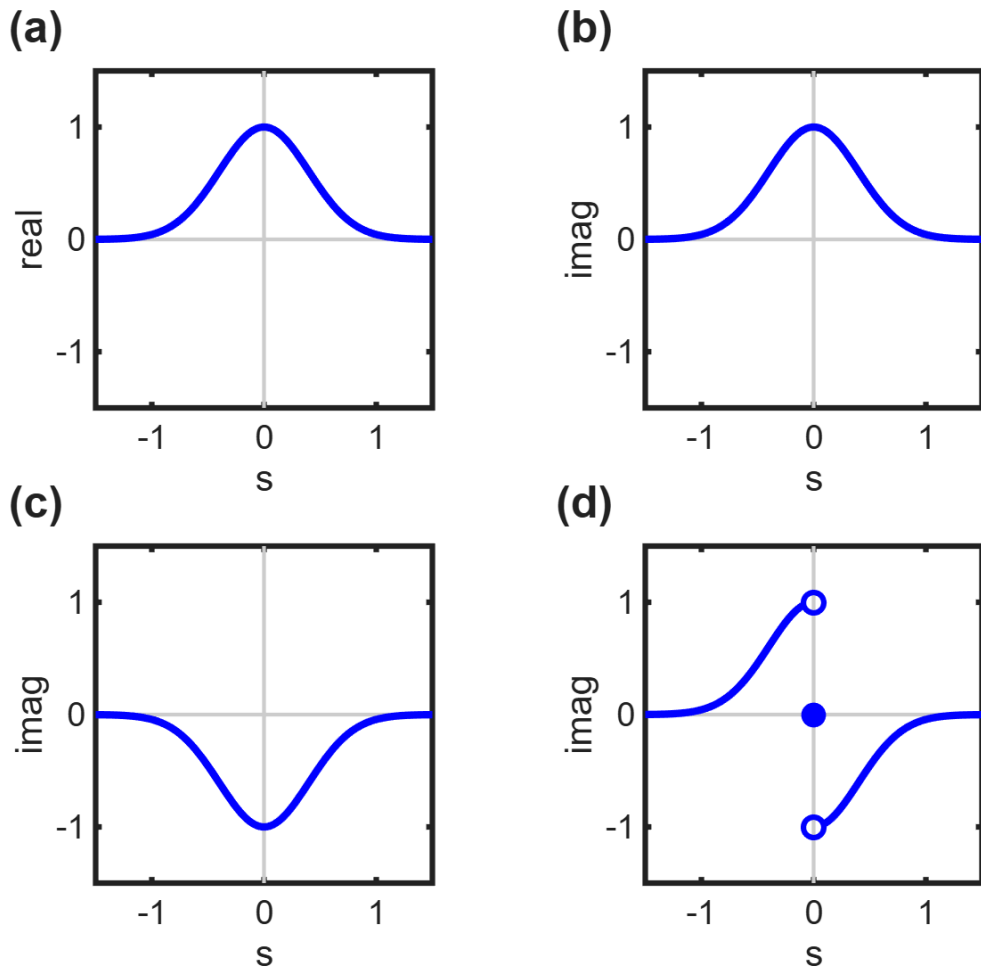


Figure 41. (a) The Fourier transform of a Gaussian. (b) The multiplication of the function in (a) by i . (c) The multiplication of the function in (b) by -1 . (d) The multiplication of the function in (c) by $\text{signum}(s)$, which gives the Fourier transform of the Hilbert transform of the Gaussian. In going from (a) to (d), the function in (a) was rotated by $+90^\circ$ or $e^{\frac{i\pi}{2}}$ for $s < 0$ and -90° or $e^{-\frac{i\pi}{2}}$ for $s > 0$.

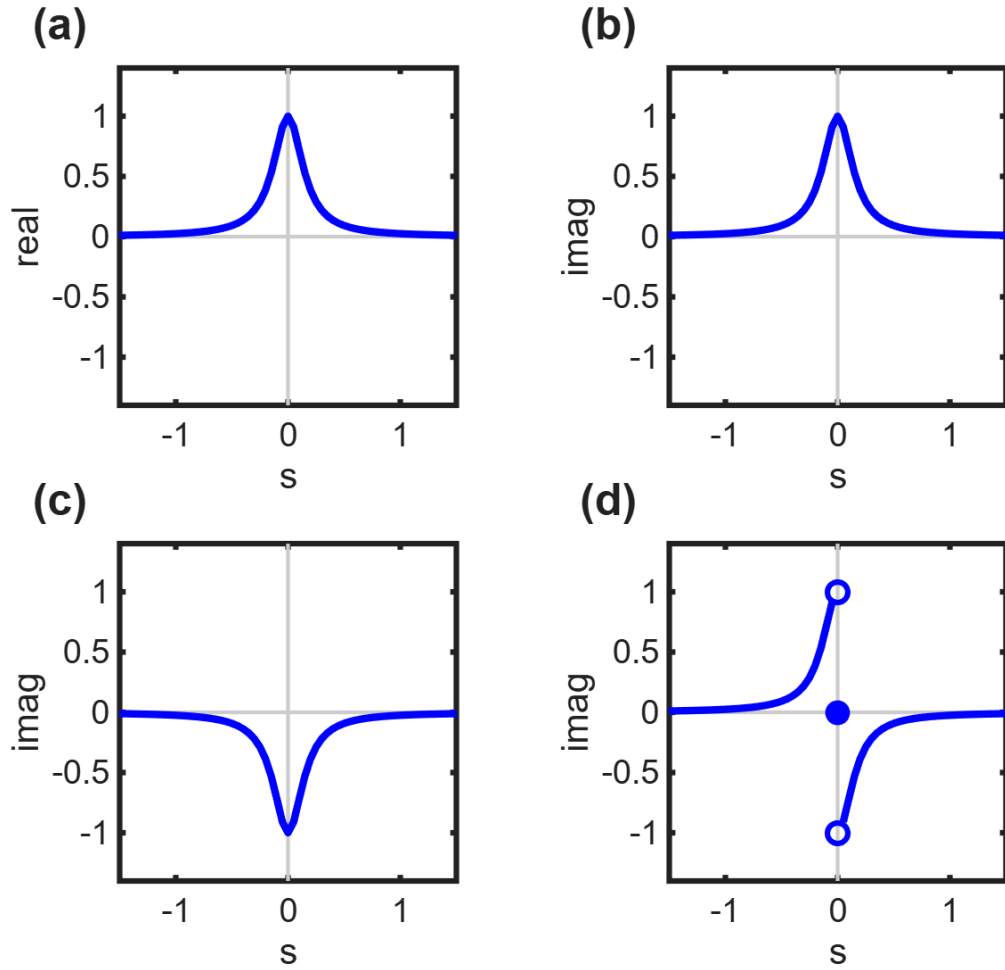


Figure 42. (a) The Fourier transform of a biexponentially decaying function, which is a Lorentzian. (b) The multiplication of the function in (a) by i . (c) The multiplication of the function in (b) by -1 . (d) The multiplication of the function in (c) by $\text{signum}(s)$, which gives the Fourier transform of the Hilbert transform of the biexponentially decaying function. In going from (a) to (d), the function in (a) was rotated by $+90^\circ$ or $e^{\frac{i\pi}{2}}$ for $s < 0$ and -90° or $e^{-\frac{i\pi}{2}}$ for $s > 0$.

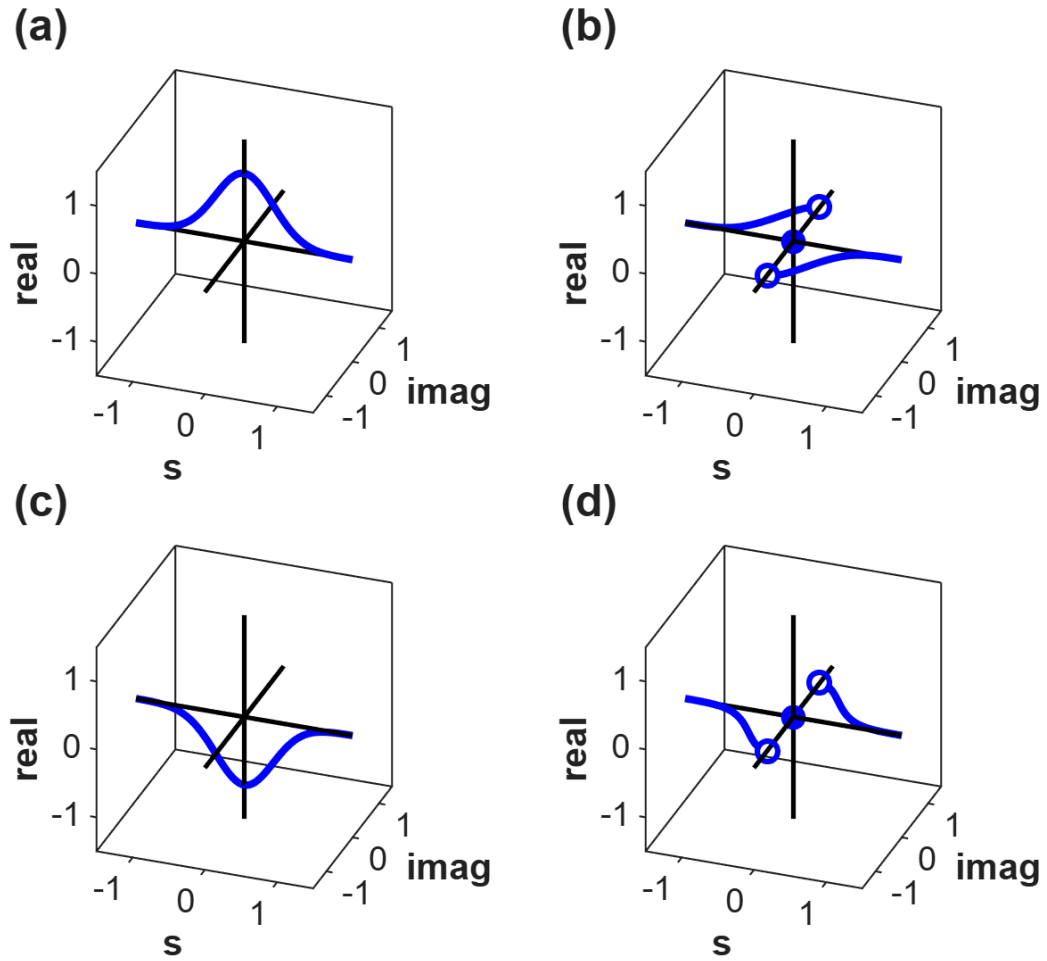


Figure 43. The reciprocal space representations of the repeated applications of the Hilbert transform to a Gaussian function. (a) the Gaussian function, (b) after the first Hilbert transform, (c) after the second Hilbert transform, (d) after the third Hilbert transform. An additional application of the Hilbert transform takes us from (d) back to (a).

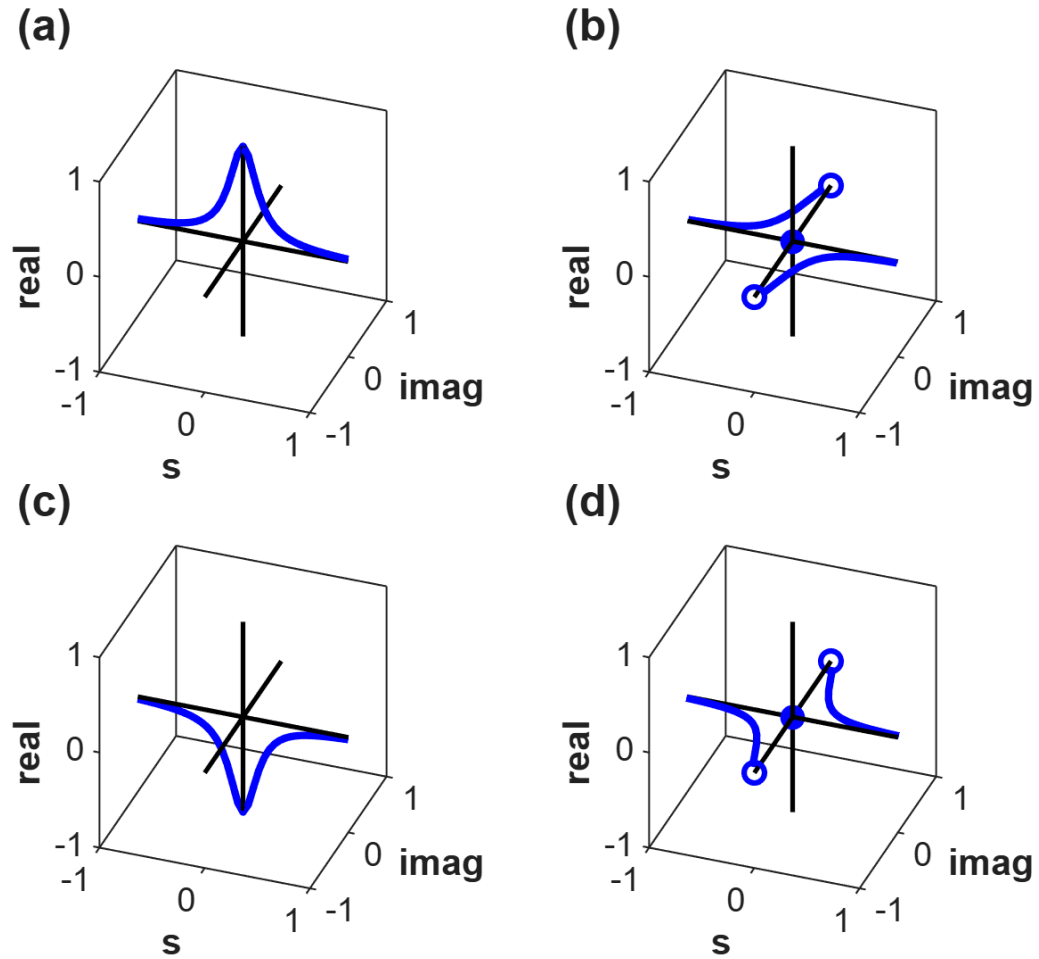


Figure 44. The reciprocal space representations of the repeated applications of the Hilbert transform to a biexponentially decaying function, which is a Lorentzian function. (a) the Lorentzian function, (b) after the first Hilbert transform, (c) after the second Hilbert transform, (d) after the third Hilbert transform. An additional application of the Hilbert transform takes us from (d) back to (a).

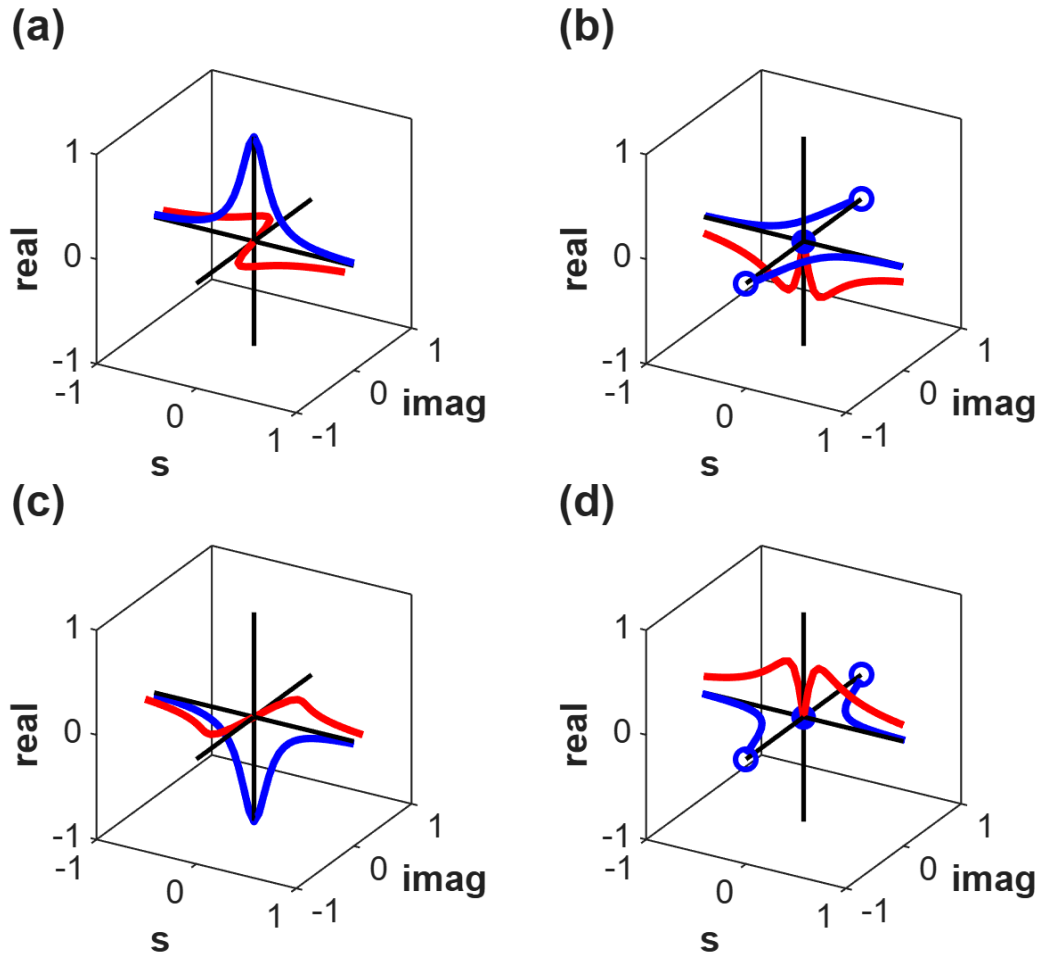


Figure 45. (a) The Fourier transform of a function $f(x)$ with $f(x) = 0$ for $x < 0$ and $f(x) = e^{-x}$ for $x > 0$, and the representations in reciprocal space of (b) one, (c) two, and (d) three Hilbert transforms of $f(x)$.

VIII. 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. Indeed, 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 $\{y_i\} = \{6, 2 + i, -5, 17\}$.

$$\{x_i\} + \{y_i\} = \{1 + 6, i + 2 + i, 4 - 5, -3 + 17\} = \{7, 2 + 2i, -1, 14\} \quad (177)$$

$$\{x_i\} - \{y_i\} = \{1 - 6, i - 2 - i, 4 + 5, -3 - 17\} = \{-5, -2, 9, -20\} \quad (178)$$

$$\{x_i\}\{y_i\} = \{1 \cdot 6, i \cdot (2 + i), 4 \cdot (-5), -3 \cdot 17\} = \{6, -1 + 2i, -20, -51\} \quad (179)$$

$$\frac{\{x_i\}}{\{y_i\}} = \left\{ \frac{1}{6}, \frac{i}{2 + i}, \frac{4}{-5}, \frac{-3}{17} \right\} = \left\{ \frac{1}{6}, \frac{1 + 2i}{5}, \frac{-4}{5}, \frac{-3}{17} \right\} \quad (180)$$

Of course, division of sequences, e.g., Equation 180, assumes that no y_i is zero.

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

$$a \{x_i\} = a \{1, i, 4, -3\} = \{a, ia, 4a, -3a\} \quad (181)$$

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 182 and 183 are based on sums, as follows:

$$C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} \quad (182)$$

$$x_n = \frac{1}{N} \sum_{k=0}^{N-1} C_k e^{i2\pi n(k/N)} \quad (183)$$

Some authors, including Bracewell³ and Weaver,⁹ place the $\frac{1}{N}$ normalization term before the sum in Equation 182 instead of as it is in this work in Equation 183. However, the DFT as defined in Equations 182 and 183 appears to be the more common way of defining currently. MATLAB uses these versions for its ‘fft’ and ‘ifft’ commands as do Walker¹² 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 182, C_0 is the sum of the entries in $\{x_n\}$. Some authors also define the DFT and inverse

DFT more symmetrically with the same $\frac{1}{\sqrt{N}}$ term in front of both equations. As is the case for the different definitions of the Fourier transform, similar, but not identical, results are obtained with the different representations of the DFT equations.

Obviously, we can expand Equations 182 and 183 using Euler's relationship as follows:

$$C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} = \sum_{n=0}^{N-1} x_n (\cos(2\pi k(n/N)) - i\sin(2\pi k(n/N))) \quad (184)$$

$$x_n = \frac{1}{N} \sum_{k=0}^{N-1} C_k e^{i2\pi n(k/N)} = \frac{1}{N} \sum_{k=0}^{N-1} C_k (\cos(2\pi k(n/N)) + i\sin(2\pi k(n/N))) \quad (185)$$

It might be assumed that because Equations 6 and 9 are based on more advanced mathematics than Equations 182 and 183 (integrals compared to sums), 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. As David Aspnes once 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 calculating the DFT with Equations 182 and 183. In general, these examples are presented as problems. Those new to DFTs will probably learn this material better by working these problems than by simply looking at their solutions.

2. *Representations of the DFT that account for the sampling interval and cycles per total sampled distance*

The definitions for the DFT given above, Equations 182 and 183, which are $C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)}$ and $x_n = \frac{1}{N} \sum_{k=0}^{N-1} C_k e^{i2\pi n(k/N)}$, are useful and practical, where the results of

these transforms (C_k and x_n , respectively) are often listed or displayed in terms of the index of the summation, i.e., $n = 0, 1, 2, \dots, N - 1$ and $k = 0, 1, 2, \dots, N - 1$. However, this approach does not explicitly take into account the positions along these functions and the frequencies of the waves considered in them. Accordingly, Equations 182 and 183 can be rewritten as:

$$C\left(\frac{k}{N\Delta x}\right) = \sum_{n=0}^{N-1} x(n\Delta x) e^{-i2\pi k(n/N)} \quad (186)$$

and

$$x(n\Delta x) = \frac{1}{N} \sum_{k=0}^{N-1} C\left(\frac{k}{N\Delta x}\right) e^{i2\pi n(k/N)} \quad (187)$$

where Δx is the sampling interval/step between data points, and $\frac{k}{N\Delta x}$ gives the number of cycles per total sampling distance.

3. *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 182 and 183, 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 presented 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., $\text{III}(x)$ (see above), which replaces $f(x)$ with a series of evenly spaced delta functions in $f(x)\text{III}(x)$ 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 $F(s) * \text{III}(s)$ in reciprocal space (recall that $\text{III}(x) \leftrightarrow \text{III}(s)$). 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 $\text{III}(x) \leftrightarrow \text{III}(s)$ suggested in this paragraph may not be the ideal 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 182 and 183, which provide a definition of the DFT based on sums. At this point, we aren't concerned how we got the definitions in Equations 182 and 183. We'll provide a deeper justification for them later.

We begin by pointing out some similarities between Equations 6 and 7 and Equations 182 and 183. 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 182 and 183, 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, and as already shown in this document, 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 and inverse DFT) as:

$$e^{-i2\pi k(n/N)} = \cos\left(2\pi k\left(\frac{n}{N}\right)\right) - i \sin\left(2\pi k\left(\frac{n}{N}\right)\right) \quad (188)$$

$$e^{i2\pi k(n/N)} = \cos\left(2\pi k\left(\frac{n}{N}\right)\right) + i \sin\left(2\pi k\left(\frac{n}{N}\right)\right) \quad (189)$$

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 182 and 183 what is going on, it is basically the same thing. In Equations 182 and 183, 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 cosine and sine functions with different frequencies. However, a key difference between the Fourier transform and the DFT is the nature of these frequencies. 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 182, $C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)}$, 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, through Euler's formula, k gives the number of cycles of the sines and cosines in $e^{-i2\pi k(n/N)}$ that fit and are sampled between $n = 0$ and $n = N - 1$.

In the DFT (Equation 182), we multiply a sequence of N data points, which we specify as: $x_0, x_1, x_2, \dots, x_{N-1}$, by an equally long sequence of values obtained by considering $n = 0, 1, 2, \dots, N - 1$ in $e^{-i2\pi k(n/N)}$ for a given value of k and sum the resulting values. This process creates a Fourier coefficient, C_k , for each value of k . The inverse DFT, Equation 183, is doing something very similar. In Equation 183, 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 plays the role of the frequency 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 182). 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. An analogous situation occurs in the inverse DFT (Equation 183) with $\frac{k}{N}$ and n .

E. Examples of Applying the DFT to sequences of numbers

Here are some examples of applying the DFT an inverse DFT to real data.

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:

$$C_k = C_0 = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} = \sum_{n=0}^1 x_n e^{-i2\pi 0(n/2)} = \sum_{n=0}^1 x_n = 0e^0 + 1e^0 = 1 \quad (190)$$

$$C_1 = \sum_{n=0}^1 x_n e^{-i2\pi 1(n/2)} = \sum_{n=0}^1 x_n e^{-i\pi n} = x_0 e^0 + x_1 e^{-i\pi} = 0 - 1 = -1 \quad (191)$$

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:

$$C_0 = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} \quad (192)$$

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

$$C_1 = \sum_{n=0}^3 x_n e^{-i2\pi 1(n/4)} \quad (193)$$

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

(194)

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

(195)

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

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

$$C_0 = \sum_{n=0}^3 x_n e^{-i2\pi 0(n/4)} = 1 \cdot e^0 + 1 \cdot e^0 + 1 \cdot e^0 + 1 \cdot e^0 = 4 \quad (196)$$

$$\begin{aligned} C_1 &= \sum_{n=0}^3 x_n e^{-i2\pi 1(n/4)} = 1 \cdot e^0 + 1 \cdot e^{-i\pi/2} + 1 \cdot e^{-i\pi} + 1 \cdot e^{-i3\pi/2} \\ &= 1 - i - 1 + i = 0 \end{aligned} \quad (197)$$

$$C_2 = \sum_{n=0}^3 x_n e^{-i\pi n} = 1 - 1 + 1 - 1 = 0 \quad (198)$$

$$C_3 = \sum_{n=0}^3 x_n e^{-i2\pi 3(n/4)} \sum_{n=0}^3 x_n e^{-i\pi n 3/2} = 1 + i - 1 - i = 0 \quad (199)$$

Thus, just like $1 \leftrightarrow \delta(x)$, the discrete Fourier transform of $\{1, 1, 1, 1\}$ is $\{4, 0, 0, 0\}$, which is the discrete analog of the delta function. That is, $\{4, 0, 0, 0\}$ is the so-called ‘delta sequence’, $\{1, 0, 0, 0\}$, multiplied by 4.

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

Solution 4. For $N = 4$ we obtain

$$C_0 = \sum_{n=0}^3 x_n e^{-i2\pi 0(n/4)} = 1 + 0 + 0 + 0 = 1 \quad (200)$$

$$C_1 = \sum_{n=0}^3 x_n e^{-i2\pi 1(n/4)} = 1 + 0 + 0 + 0 = 1 \quad (201)$$

$$C_2 = \sum_{n=0}^3 x_n e^{-i2\pi 2(n/4)} = 1 + 0 + 0 + 0 = 1 \quad (202)$$

$$C_3 = \sum_{n=0}^3 x_n e^{-i2\pi 3(n/4)} = 1 + 0 + 0 + 0 = 1 \quad (203)$$

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 ($\delta(x) \leftrightarrow 1$).

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 $\{C_k\}_{k=0}^{N-1} = \{1, 1, 1, \dots, 1\}$.

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:

$$x_n = x_0 = \frac{1}{N} \sum_{k=0}^{N-1} C_k e^{i2\pi n(k/N)} \quad (204)$$

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

$$x_1 = \frac{1}{2} \sum_{k=0}^1 C_k e^{i2\pi 1k/2} = \frac{1}{2} (1 \cdot e^0 + (-1) \cdot e^{i\pi}) = 1 \quad (205)$$

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 183 we obtain:

$$x_0 = \frac{1}{4} \sum_{k=0}^3 C_k e^{i2\pi 0(k/4)} = \frac{1}{4} (7 \cdot e^0 + (-2 - i) \cdot e^0 + 1 \cdot e^0 + (-2 + i) \cdot e^0) \quad (206)$$

$$= 1$$

$$x_1 = \frac{1}{4} \sum_{k=0}^3 C_k e^{i2\pi 1(k/4)} \quad (207)$$

$$= \frac{1}{4} (7 \cdot e^{i2\pi 1(0/4)} + (-2 - i) \cdot e^{i2\pi 1(1/4)} + 1 \cdot e^{i2\pi 1(2/4)} + (-2 + i) \cdot e^{i2\pi 1(3/4)})$$

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

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

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

$$x_2 = \frac{1}{4} \sum_{k=0}^3 C_k e^{i2\pi 2(k/4)} \quad (208)$$

$$= \frac{1}{4} (7 \cdot e^{0\pi} + (-2 - i) \cdot e^{i\pi} + 1 \cdot e^{i2\pi} + (-2 + i) \cdot e^{i3\pi})$$

$$= \frac{1}{4} (7 + (-2 - i)(-1) + 1 \cdot 1 + (-2 + i) \cdot (-1)) = 3$$

$$\begin{aligned}
x_3 &= \frac{1}{4} \sum_{k=0}^3 C_k e^{i2\pi 3(k/4)} \tag{209} \\
&= \frac{1}{4} (7 \cdot e^0 + (-2 - i) \cdot e^{i\pi(3/2)} + 1 \cdot e^{i3\pi} + (-2 + i) \cdot e^{i\pi(9/2)}) \\
&= \frac{1}{4} (7 + (-2 - i) \cdot (-i) + 1 \cdot (-1) + (-2 + i) \cdot i) = 1
\end{aligned}$$

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 begin by using Euler's relationship to break Equation 182 into its real and imaginary parts.

$$C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} = \sum_{n=0}^{N-1} x_n \cos\left(2\pi k \left(\frac{n}{N}\right)\right) - i \sum_{n=0}^{N-1} x_n \sin\left(2\pi k \left(\frac{n}{N}\right)\right) \tag{210}$$

We now write out Equation 210 in Equation 211 for an arbitrary value of k and $N = 8$. That is, Equation 211 shows results for $\frac{n}{N} = \frac{n}{8}$ for $n = 0, 1 \dots 7$. Equation 211 is a sampling at equal intervals across sines and cosines with frequencies k .

$$\begin{aligned}
C_k = & x_0 \cos\left(2\pi k \left(\frac{0}{8}\right)\right) + x_1 \cos\left(2\pi k \left(\frac{1}{8}\right)\right) + x_2 \cos\left(2\pi k \left(\frac{2}{8}\right)\right) \\
& + x_3 \cos\left(2\pi k \left(\frac{3}{8}\right)\right) + x_4 \cos\left(2\pi k \left(\frac{4}{8}\right)\right) + x_5 \cos\left(2\pi k \left(\frac{5}{8}\right)\right) \\
& + x_6 \cos\left(2\pi k \left(\frac{6}{8}\right)\right) \\
& + x_7 \cos\left(2\pi k \left(\frac{7}{8}\right)\right) \\
& - i \left(x_0 \sin\left(2\pi k \left(\frac{0}{8}\right)\right) + x_1 \sin\left(2\pi k \left(\frac{1}{8}\right)\right) + x_2 \sin\left(2\pi k \left(\frac{2}{8}\right)\right) \right. \\
& + x_3 \sin\left(2\pi k \left(\frac{3}{8}\right)\right) + x_4 \sin\left(2\pi k \left(\frac{4}{8}\right)\right) + x_5 \sin\left(2\pi k \left(\frac{5}{8}\right)\right) \\
& \left. + x_6 \sin\left(2\pi k \left(\frac{6}{8}\right)\right) + x_7 \sin\left(2\pi k \left(\frac{7}{8}\right)\right) \right)
\end{aligned} \tag{211}$$

For $N = 32$, Figure 46 - Figure 48 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, the lower-index Fourier coefficients, C_k , are the result of multiplications of our sequence 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.

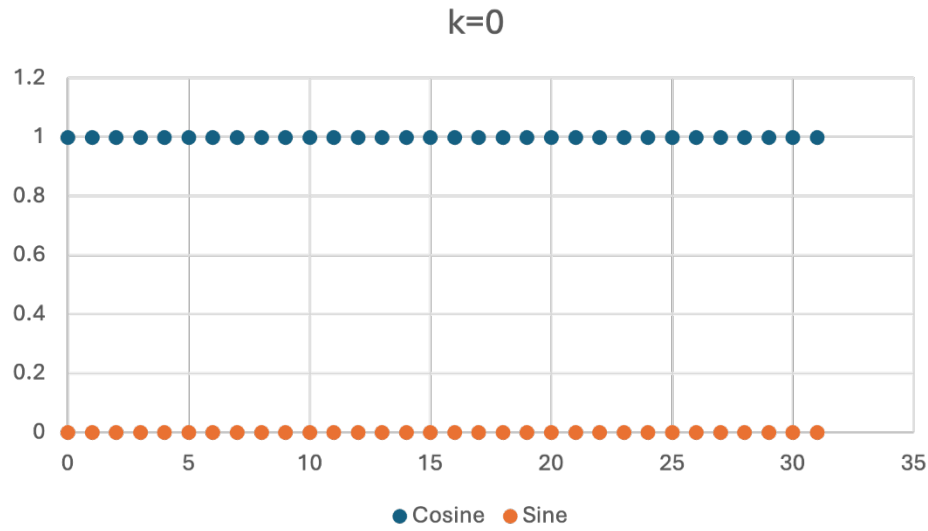


Figure 46. The cosine and sine ‘waves’ with $k = 0$ that are multiplied by a sequence of 32 data points ($N = 32$) in a DFT to produce C_0 as described in Equation 210.

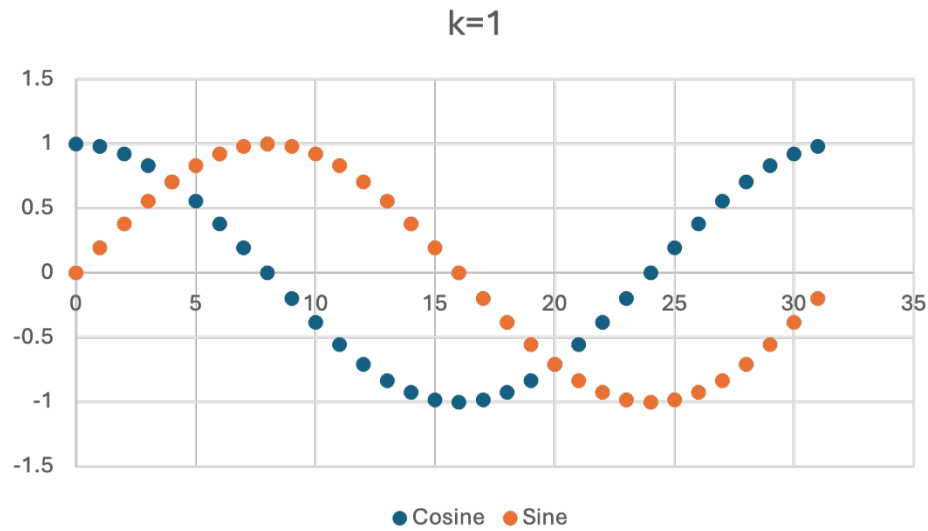


Figure 47. The cosine and sine waves with $k = 1$ that are multiplied by a sequence of 32 data points ($N = 32$) in a DFT to produce C_1 as described in Equation 210. That is, $k = 1$ corresponds to 1 cycle of the waves across the 32 data points.

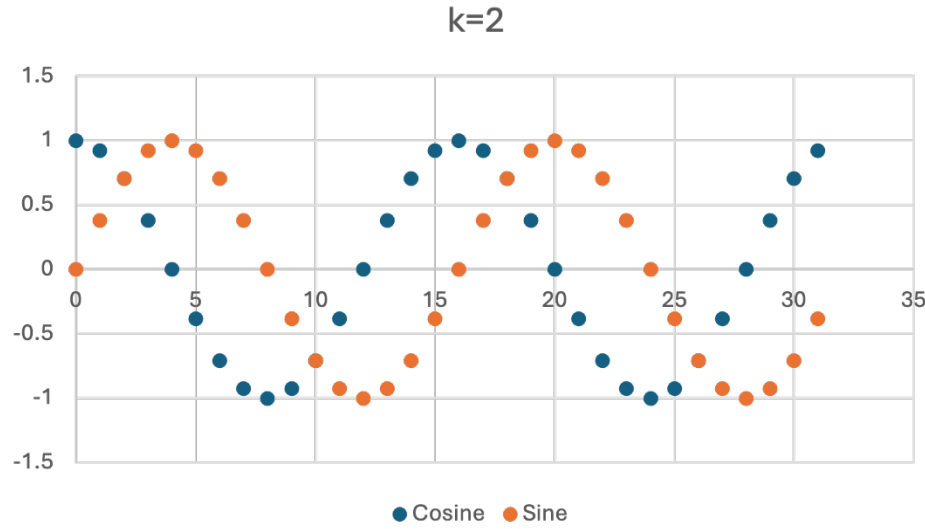


Figure 48. The cosine and sine waves with $k = 2$ that are multiplied by a sequence of 32 data points ($N = 32$) in a DFT to produce C_2 as described in Equation 210. That is, $k = 2$ corresponds to 2 cycles of the waves across the 32 data points.

G. Rewriting the DFT as a matrix

Of course, as we did above, it is valid to write the DFT as a sum. However, it can be more useful to consider it as a matrix algebra problem. We now rewrite and solve the first four examples above in matrix algebra form and then comment on what we have done.

1. Matrix algebra reformulation of the DFT

Here we use matrix algebra to resolve the first four examples given above of finding the DFTs of some short sequences of numbers.

Example 1. Take the DFT of $\{0, 1\}$ using a matrix algebra representation of the DFT.

Solution 1. We can rewrite what we have above as:

$$C_0 = \sum_{n=0}^{N-1} x_n e^{-i2\pi 0(n/N)} = x_0 e^{-i2\pi 0(0/N)} + x_1 e^{-i2\pi 0(1/N)} \quad (212)$$

$$C_1 = \sum_{n=0}^1 x_n e^{-i2\pi 1(n/2)} = x_0 e^{-i2\pi 1(0/2)} + x_1 e^{-i2\pi 1(1/2)} \quad (213)$$

And then rewrite these equations in matrix form as

$$\begin{bmatrix} C_0 \\ C_1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \quad (214)$$

Thus, for this problem:

$$\begin{bmatrix} C_0 \\ C_1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (215)$$

Example 2. Calculate the DFT of a longer sequence of numbers: $\{1, 2, 3, 1\}$ using a matrix algebra representation of the DFT.

Solution 2. We express this problem as:

$$\begin{aligned} C_0 &= \sum_{n=0}^{N-1} x_n e^{-i2\pi 0(n/N)} \\ &= x_0 e^{-i2\pi 0(0/4)} + x_1 e^{-i2\pi 0(1/4)} + x_2 e^{-i2\pi 0(2/4)} + x_3 e^{-i2\pi 0(3/4)} \end{aligned} \quad (216)$$

$$C_1 = \sum_{n=0}^3 x_n e^{-i2\pi 1(n/4)} \quad (217)$$

$$= x_0 e^{-i2\pi 1(0/4)} + x_1 e^{-i2\pi 1(1/4)} + x_2 e^{-i2\pi 1(2/4)} + x_3 e^{-i2\pi 1(3/4)} \quad (218)$$

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

$$= x_0 e^{-i2\pi 2(0/4)} + x_1 e^{-i2\pi 2(1/4)} + x_2 e^{-i2\pi 2(2/4)} + x_3 e^{-i2\pi 2(3/4)} \quad (219)$$

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

$$= x_0 e^{-i2\pi 3(0/4)} + x_1 e^{-i2\pi 3(1/4)} + x_2 e^{-i2\pi 3(2/4)} + x_3 e^{-i2\pi 3(3/4)}$$

which we can write as:

$$\begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \end{bmatrix} = \begin{bmatrix} e^{-i2\pi 0(0/4)} & e^{-i2\pi 0(1/4)} & e^{-i2\pi 0(2/4)} & e^{-i2\pi 0(3/4)} \\ e^{-i2\pi 1(0/4)} & e^{-i2\pi 1(1/4)} & e^{-i2\pi 1(2/4)} & e^{-i2\pi 1(3/4)} \\ e^{-i2\pi 2(0/4)} & e^{-i2\pi 2(1/4)} & e^{-i2\pi 2(2/4)} & e^{-i2\pi 2(3/4)} \\ e^{-i2\pi 3(0/4)} & e^{-i2\pi 3(1/4)} & e^{-i2\pi 3(2/4)} & e^{-i2\pi 3(3/4)} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad (220)$$

$$= \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} 7 \\ -2 - i \\ 1 \\ -2 + i \end{bmatrix}$$

Example 3. Calculate the DFT of $\{1, 1, 1, 1\}$ using a matrix algebra representation of the DFT.

Solution 3. Now that we have the matrix that represents the DFT for a fourth-order sequence, we can simply write:

$$\begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 4 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (221)$$

Example 4. Calculate the DFT of the delta sequence, $\{1, 0, 0, 0\}$ using a matrix algebra representation of the DFT.

Solution 4. Again, using the DFT matrix for a fourth-order sequence we obtain

$$\begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad (222)$$

We can similarly represent the inverse DFT as a matrix.

2. *Comments on what we have just done*

Here are a few observations on what we just did, which include a comparison between Fourier analysis and principal component analysis (PCA), where the latter is a widely used data science method.

- i. The matrix algebra version of the DFT can be easier to implement than the version based on the sum. Once we generated the DFT matrix for a fourth-order sequence in Example 2, we could immediately apply this matrix in Examples 3 and 4.
- ii. In these matrix calculations, $N \times N = N^2$ multiplications are necessary. That is, the speed of these matrix calculations goes as $\mathcal{O}(N^2)$, where $\mathcal{O}$ stands for ‘order’. Thus, for large data sets, the DFT can become difficult or impractical to perform. A much better algorithm for calculating discrete Fourier transforms is the so-called Fast Fourier Transform (FFT) algorithm.
- iii. The rows and columns of the DFT matrices are orthogonal to each other with respect to the conjugate inner product. That is, $row_i \cdot row_j^* = 0$ or $column_i \cdot column_j^* = 0$ for $i \neq j$.
- iv. While both are important in data analysis/data science, principal component analysis (PCA) and the DFT are fundamentally different ways of handling and understanding data. In PCA, a model is created from a group of spectra. The model depends on and is a result of the spectra. In contrast, in the DFT, a spectrum is multiplied by a series of orthogonal vectors/sinusoids, which were not created from the spectrum in question or a group of spectra. That is, the DFT can be seen as a projection of a spectrum onto a set of predetermined, orthogonal vectors, where, again, these orthogonal vectors are not derived from a group of spectra as they are in PCA. (As an aside, at a recent conference, Linford was asked by someone who is familiar with PCA, but not with Fourier analysis, how many spectra are required to create a model in Fourier analysis. The answer is only one, which is an obvious advantage of the Fourier approach.)

H. *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 182:

$$\begin{aligned}
 C_{k+N} &= \sum_{n=0}^{N-1} x_n e^{-i2\pi(k+N)(n/N)} \\
 &= \sum_{n=0}^{N-1} x_n e^{-i2\pi(kn/N)} e^{-i2\pi n} = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)} = C_k
 \end{aligned} \tag{223}$$

Equation 223 is valid because n is an integer in $e^{-i2\pi n}$. Furthermore, even though spectra from analytical instruments are not infinitely periodic, or even periodic in any way, they turn out to be periodic in the DFT when we consider $x_n = x_{n+N}$, as follows:

$$\begin{aligned}
 x_{n+N} &= \frac{1}{N} \sum_{k=0}^{N-1} C_k e^{i2\pi(n+N)(k/N)} = \frac{1}{N} \sum_{k=0}^{N-1} C_k e^{i2\pi n(k/N)} e^{i2\pi k} \\
 &= \frac{1}{N} \sum_{k=0}^{N-1} C_k e^{i2\pi n(k/N)} = x_n
 \end{aligned} \tag{224}$$

This relationship again holds because k is an integer in $e^{i2\pi k}$. In summary, even though the DFT is performed on a finite sequence of numbers, both C_k and x_n can be considered to be periodic (and mathematically speaking actually are periodic) in it.

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 de facto 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: $\dots, 2, -3, 4, 5, 5, 4, -3, \underline{2}, -3, 4, 5, 5, 4, -3 \dots$, where x_0 , which is 2, is bolded and underlined. We note that $x_1 = x_{-1} = -3$, where also because of the periodicity of the DFT, $x_1 = x_{-1} = x_{N-1} = x_6 = -3$. Similarly, $x_2 = x_{-2} = x_{N-2} = x_5 = 4$, etc. The first element, x_0 , in an even sequence can have any value because, for $i = 0$, it is always the case that $x_i = x_{-i} = x_0$.

The following sequence is odd: $\{0, -3, 4, 5, -5, -4, 3\}$. Note that, unlike with even sequences, the first element, x_0 , in an odd sequence must be zero. That is, $x_0 = 0$ 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 write part of its periodic extension: $\dots, \underline{0}, -3, 4, 5, -5, -4, 3, \underline{0}, -3, 4, 5, -5, -4, 3, \dots$ and note that $x_1 = -x_{-1} = -x_{N-1} = -x_6 = -3$, $x_2 = -x_{-2} = -x_{N-2} = -x_5 = 4$, etc.

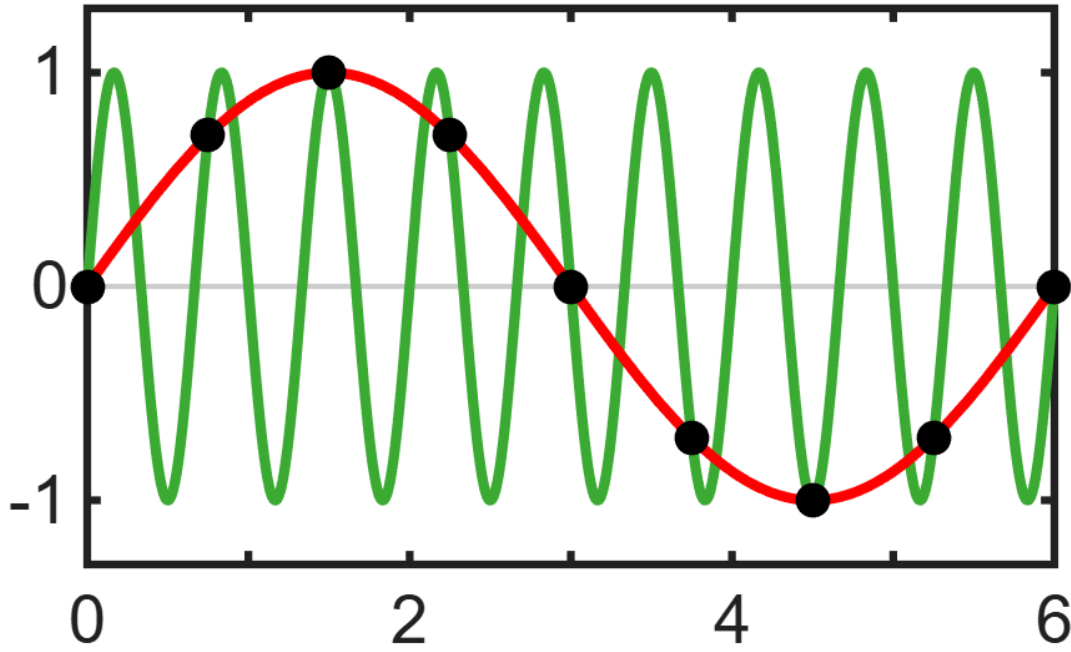


Figure 49. An illustration of aliasing. A set of equally spaced, sampled points along the x -axis has the same values for two different cosines: $\cos\left(2\pi \cdot 1 \cdot \left(\frac{n}{8}\right)\right)$ and $\cos\left(2\pi \cdot 9 \cdot \left(\frac{n}{8}\right)\right)$ for $n = 1, 2, \dots, 7, 8, \dots$, which makes distinguishing between the results of these cosines in the DFT impossible.

3. Aliasing

As just shown, the Fourier coefficients and reconstructed sample sequence are periodic in the DFT, i.e., $C_k = C_{k+N}$ and $x_n = x_{n+N}$. However, this fact does more than allow us to regard both the Fourier coefficients and values of the original sequence as periodic, it introduces a fundamental ambiguity into the DFT, which is known as aliasing. Aliasing arises because of sampling, which is why it is not present in the Fourier transforms of continuous functions. That is, for the DFT and because $C_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k(n/N)}$, $C_{k+N} = \sum_{n=0}^{N-1} x_n e^{-i2\pi(k+N)(n/N)}$, and, for that matter, $C_k = C_{k+pN} = \sum_{n=0}^{N-1} x_n e^{-i2\pi(k+pN)(n/N)}$, where p is an integer, there is always some mathematical ambiguity associated with the frequency that produced the results in the DFT. These concepts are illustrated in Figure 49. For example, Figure 49 shows the real part of $e^{-i2\pi k(n/N)}$ for

C_1 for a sequence of order 8, which is $\cos\left(2\pi k \left(\frac{n}{N}\right)\right) = \cos\left(2\pi \cdot 1 \cdot \left(\frac{n}{8}\right)\right)$, where the values of this function at $n = 0, 1, 2, \dots, 7$ are indicated by points (the point at $n = 8$ is also shown). This figure also shows the real part of $e^{-i2\pi \cdot 9(n/8)}$, i.e., $\cos\left(2\pi \cdot 9 \cdot \left(\frac{n}{8}\right)\right)$, for C_9 . Notice that these cosines have the same values at the sampled points. This will also be the case for C_2 and C_{10} , C_3 and C_{11} , etc. Thus, an infinite number of Fourier coefficients in the DFT have the same values, i.e., $C_k = C_{k+pN}$, which creates an ambiguity. This phenomenon is called aliasing because, in the DFT, sinusoids of different frequencies are indistinguishable from another.

While aliasing is of fundamental importance in the DFT, it is not a significant issue in the practical denoising of XPS spectra. When viewing the Fourier coefficients of most XPS spectra, it is quite reasonable to assume that the lower-index Fourier coefficients correspond to signal and that higher-index Fourier coefficients correspond to noise.

I. ***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 can be 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 used with 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 $W_N^+ = e^{i2\pi/N}$, 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:

$$C_k = \sum_{n=0}^{N-1} x_n W_N^{-nk} \quad (225)$$

$$x_n = \frac{1}{N} \sum_{k=0}^{N-1} C_k W_N^{nk} \quad (226)$$

J. *Confirming the Reversibility of the DFT Equation*

1. *The sum of a finite geometric series*

The key result in this section is a proof that relies on a result that we now derive, which is the sum of a finite geometric series. To derive this sum, where this derivation is well-known, we consider the following two geometric series,

$$S = 1 + r + r^2 + \dots + r^{N-1} \quad (227)$$

$$rS = r + r^2 + r^3 + \dots + r^N \quad (228)$$

We now subtract rS from S to obtain:

$$S - rS = S(1 - r) = 1 - r^N \quad (229)$$

Solving for S gives us:

$$S = \frac{1 - r^N}{1 - r} \quad (230)$$

2. Reversibility/reciprocity of the DFT Equations

We defined the DFT using W_N ($e^{i2\pi/N}$) in Equations 225 and 226. 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 182, we uniquely obtain the same sequence back through Equation 183.

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

$$x_n = \frac{1}{N} \sum_{k=0}^{N-1} C_k W_N^{nk} = \frac{1}{N} \sum_{k=0}^{N-1} \left[\sum_{j=0}^{N-1} x_j W_N^{-jk} \right] W_N^{nk} \quad (231)$$

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

$$x_n = \frac{1}{N} \sum_{k=0}^{N-1} C_k W_N^{nk} = \frac{1}{N} \sum_{j=0}^{N-1} x_j \sum_{k=0}^{N-1} W_N^{-jk} W_N^{nk} = \frac{1}{N} \sum_{j=0}^{N-1} x_j \sum_{k=0}^{N-1} W_N^{(n-j)k} \quad (232)$$

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

$$\begin{aligned} x_n &= \frac{1}{N} \sum_{k=0}^{N-1} C_k W_N^{nk} \\ &= \frac{1}{N} \sum_{j=0}^{N-1} x_j \sum_{k=0}^{N-1} W_N^{(n-j)k} \\ &= \frac{1}{N} (x_0 \sum_{k=0}^{N-1} W_N^{(n-0)k} + x_1 \sum_{k=0}^{N-1} W_N^{(n-1)k} + \dots \\ &\quad + x_n \sum_{k=0}^{N-1} W_N^{(n-n)k} + \dots + x_{N-1} \sum_{k=0}^{N-1} W_N^{(n-(N-1))k} + \dots) \end{aligned} \quad (233)$$

Now, there are two possibilities for $n - j$ in Equation 232. 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:

$$\begin{aligned} \sum_{k=0}^{N-1} W_N^{(n-j)k} &= 1 + \left(W_N^{(n-j)}\right)^1 + \left(W_N^{(n-j)}\right)^2 + \dots + \left(W_N^{(n-j)}\right)^{N-1} \\ &= \frac{1 - \left(W_N^{(n-j)}\right)^N}{1 - W_N^{(n-j)}} \end{aligned} \quad (234)$$

However, $W_N = e^{i2\pi/N}$ so $\left(W_N^{(n-j)}\right)^N = \left(e^{i2\pi(n-j)/N}\right)^N = e^{i2\pi(n-j)} = 1$. Thus,

$\sum_{k=0}^{N-1} W_N^{(n-j)k} = \frac{1 - \left(W_N^{(n-j)}\right)^N}{1 - W_N^{(n-j)}} = \frac{1-1}{1-W_N^{(n-j)}} = 0$. Thus, every term in Equation 232 for which $j \neq n$

disappears, leaving us:

$$\begin{aligned} x_n &= \frac{1}{N} \sum_{k=0}^{N-1} C_k W_N^{nk} = \frac{1}{N} \sum_{j=0}^{N-1} x_j \sum_{k=0}^{N-1} W_N^{(n-j)k} = \frac{1}{N} \left(x_n \sum_{k=0}^{N-1} W_N^{(n-n)k} \right) \\ &= \frac{1}{N} \left(x_n \sum_{k=0}^{N-1} 1 \right) = \frac{1}{N} x_n N = x_n \end{aligned} \quad (235)$$

which completes our proof.

K. *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 simply defines a variable by writing it at the command line (`>>`) and associating it with a mathematical operation. Also, 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.

A broader Gaussian (Figure 50) was created in MATLAB using the following code:

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

(236)

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’.

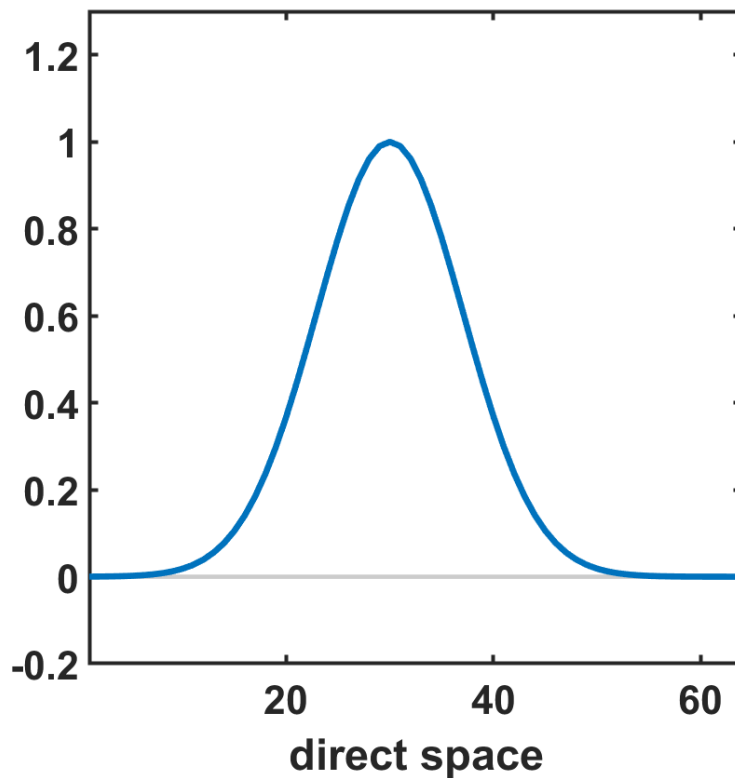


Figure 50. A broader Gaussian based on 64 data points. See Equation 236 for the MATLAB code used to make it.

We now take the DFT of `yvals` in Equation 236 and plot the real and imaginary parts of it. The MATLAB command for taking the DFT is `fft`.

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

(237)

Next, we take the real part of `fft_yvals` from Equation 237 and plot it (see Figure 51) using the commands:

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

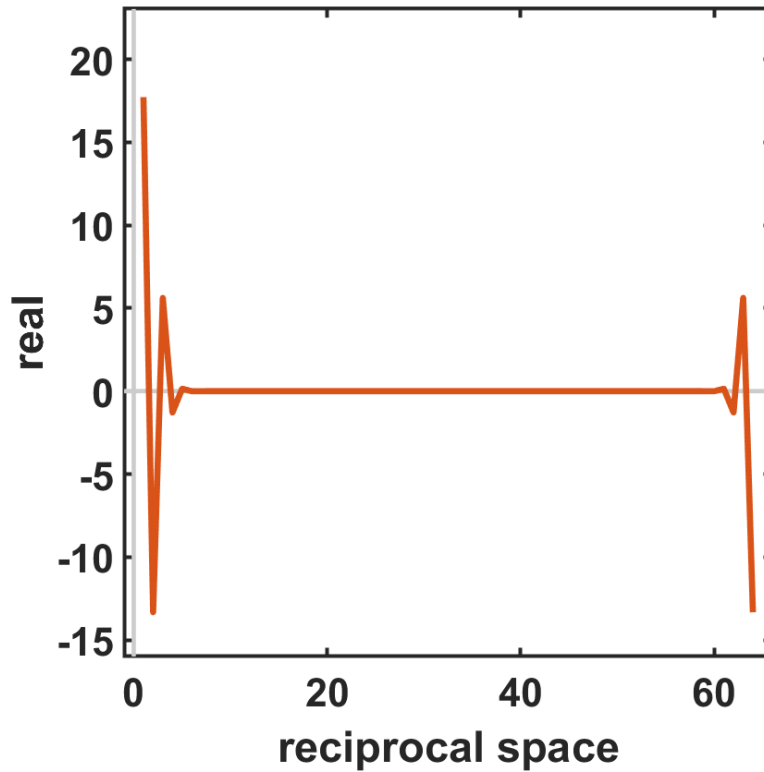
(238)

Figure 51. The real part of the DFT of the Gaussian shown in Figure 50 generated with the commands in Equation 238.

And we then take the imaginary part of `fft_yvals` and plot it (Figure 52) using the following commands:

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

(239)

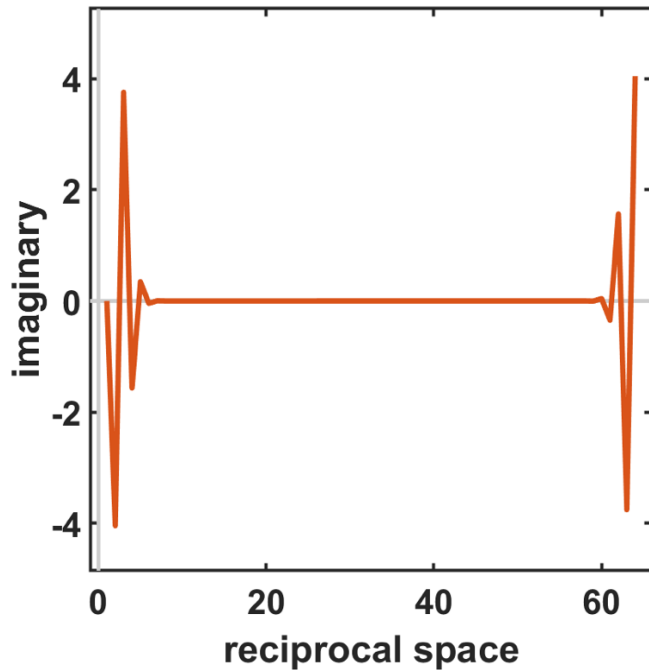


Figure 52. The imaginary part of the DFT of the Gaussian shown in Figure 50 generated with the commands in Equation 239.

While Figure 51 and Figure 52 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 53 as follows:

```
>> fft_yvals_mod = sqrt(fft_yvals_real.^2 + fft_yvals_imag.^2)    (240)
>> plot(xvals, fft_yvals_mod), shg
```

The phase, which is the arctan of the imaginary part of the DFT divided by its real part, may or may not be displayed. 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. 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`.

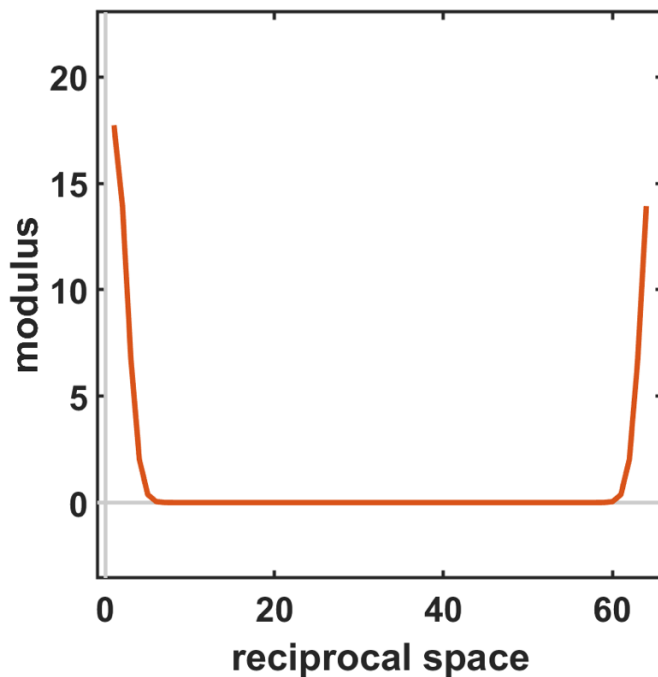


Figure 53. The modulus of the DFT of the broader Gaussian shown in Figure 50 generated with the commands in Equation 240.

We now create a narrower Gaussian than the one in Example 1 (Figure 50) and examine its DFT. Figure 54 shows this narrower Gaussian, and Figure 55 shows the modulus of its DFT, which were made as follows:

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

(241)

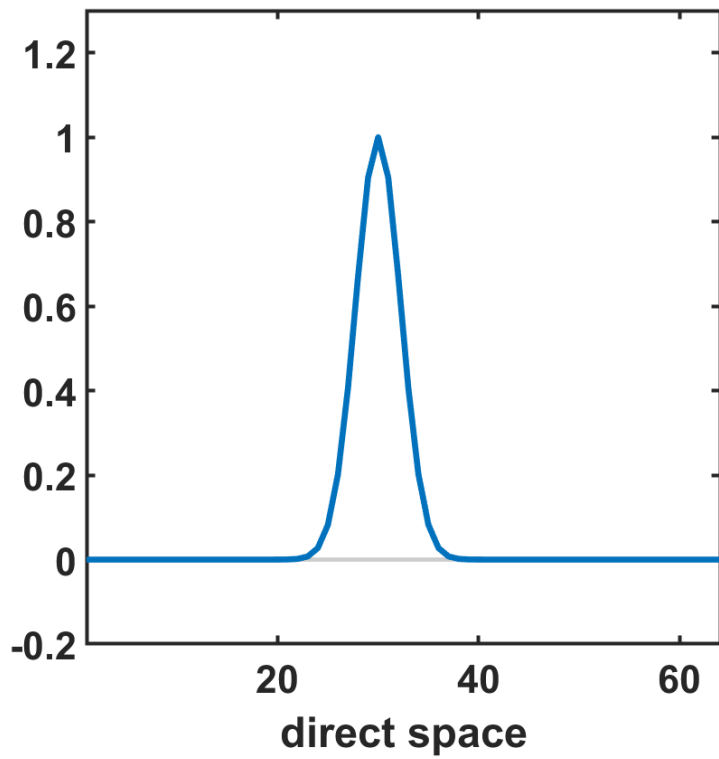


Figure 54. A narrower Gaussian based on 64 data points. See Equation 241 for the MATLAB code used to make it.

We now take the DFT of this narrower Gaussian and plot its modulus in Figure 55, as follows:

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

(242)

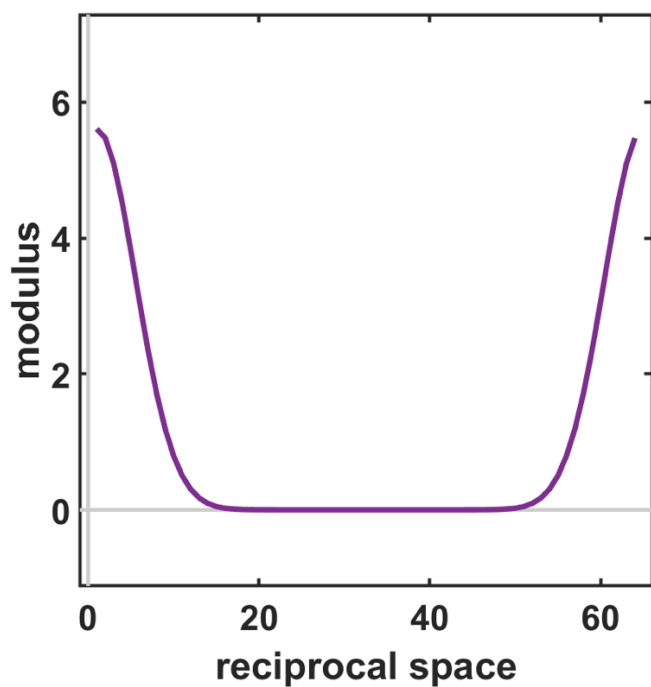


Figure 55. The modulus of the DFT of the Gaussian shown in Figure 54 generated with the commands in Equation 242.

Figure 56 shows a plot of the moduli of the DFTs of the broader (Figure 50) and narrower (Figure 54) 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 a broader Gaussian.

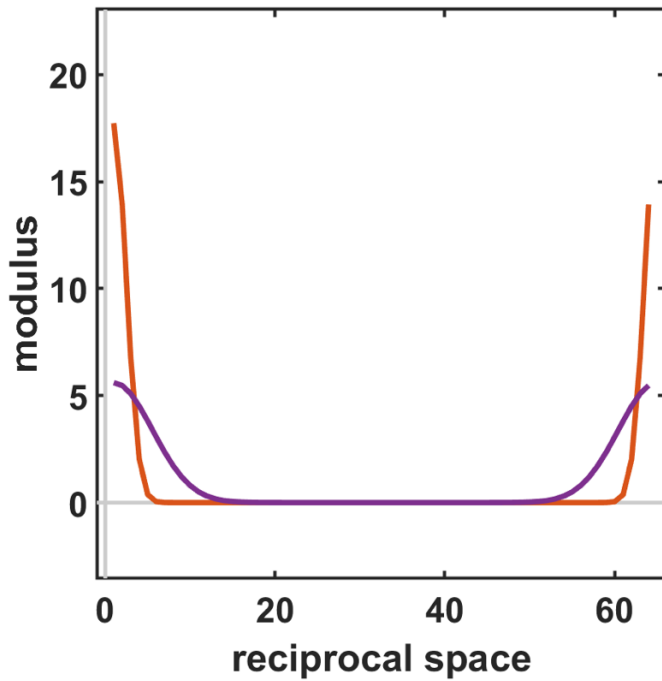


Figure 56. The moduli of the DFTs of the broader (Figure 50) and narrower (Figure 54) Gaussians just created and discussed, which are orange and purple, respectively. That is, the DFT of the broader Gaussian is narrower.

L. 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 50 and calculate its DFT. That is, we add normally distributed, random numbers to the peak contained in `yvals` (the peak in Figure 50) as follows:

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

(243)

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

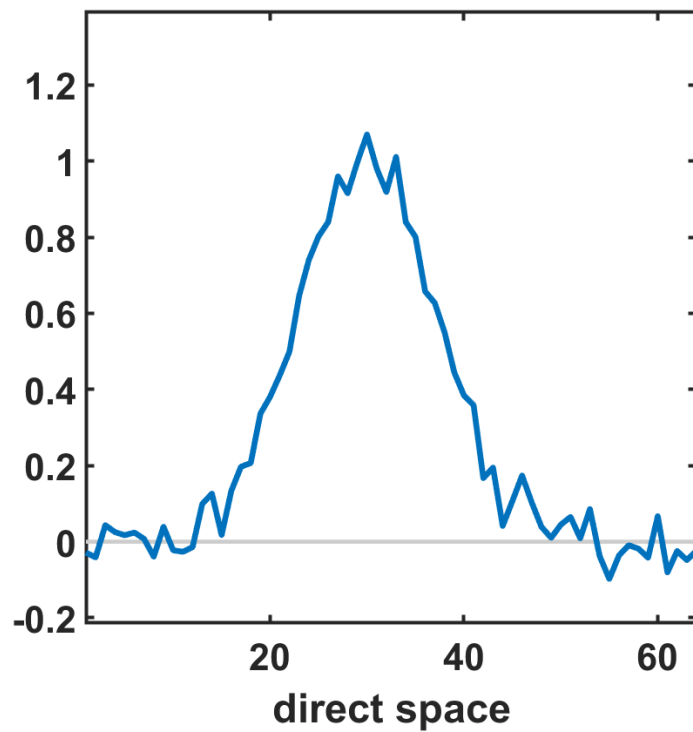


Figure 57. The Gaussian peak in Figure 50 with random noise added to it. See Equation 243.

We now take the modulus (abs) of the DFT (fft) of the data in Figure 57 and plot it in Figure 58, as follows:

```
>> plot(xvals, abs(fft(yvals_noise))), shg (244)
```

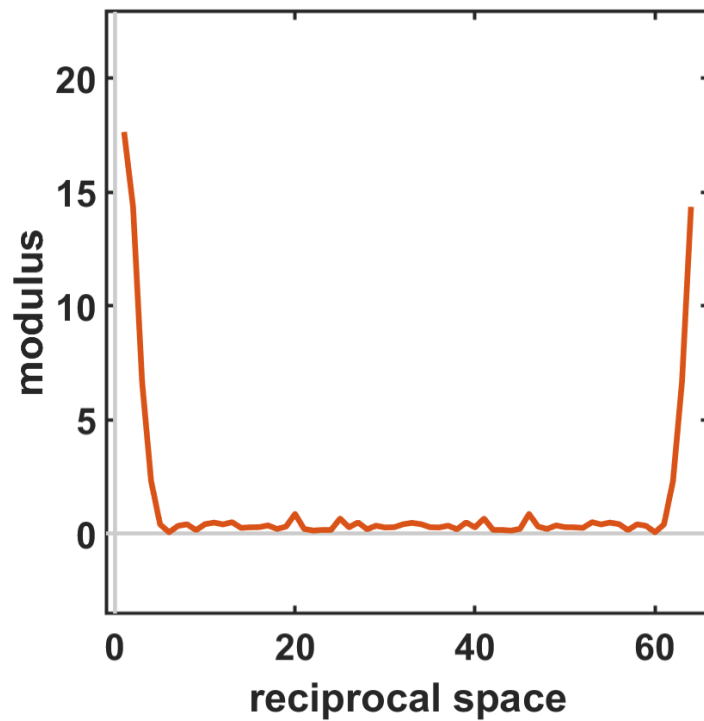


Figure 58. Modulus of the DFT of the noisy Gaussian in Figure 57.

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

In Figure 59, we overlay the moduli of the Fourier coefficients of the noisy (Figure 58) and noise-free (Figure 53) broader Gaussians using the following code:

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

(245)

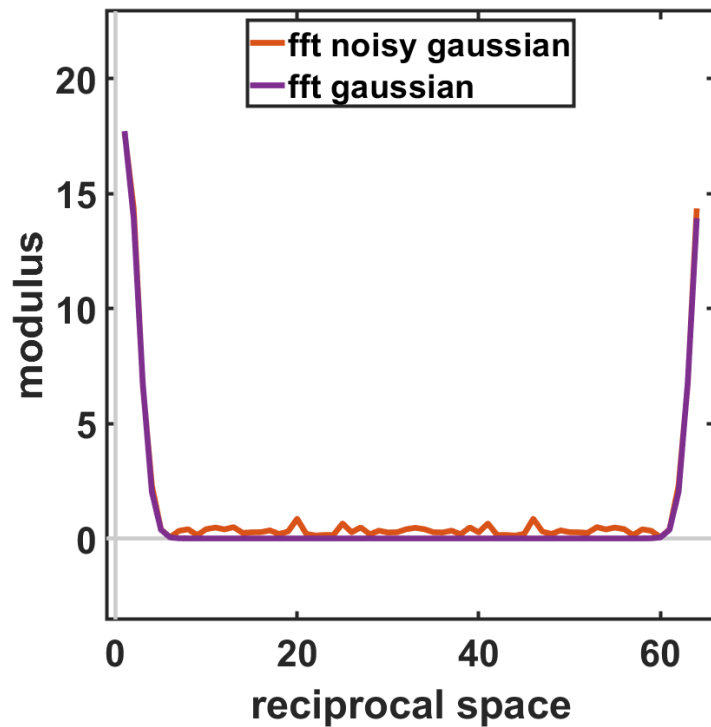


Figure 59. Overlay of the moduli of the DFTs of the Gaussians in Figure 53 and Figure 58.

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 60 and Figure 61, respectively, where the following segments of code were used:

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

(246)

and

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

(247)

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

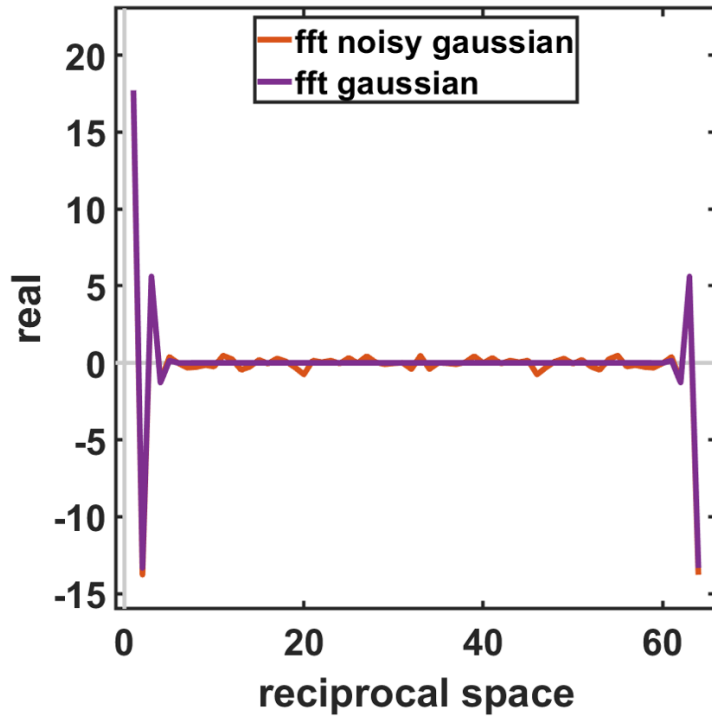


Figure 60. Real parts of the DFTs of the broader, noise-free and noisy Gaussians in Figure 50 and Figure 57, respectively.

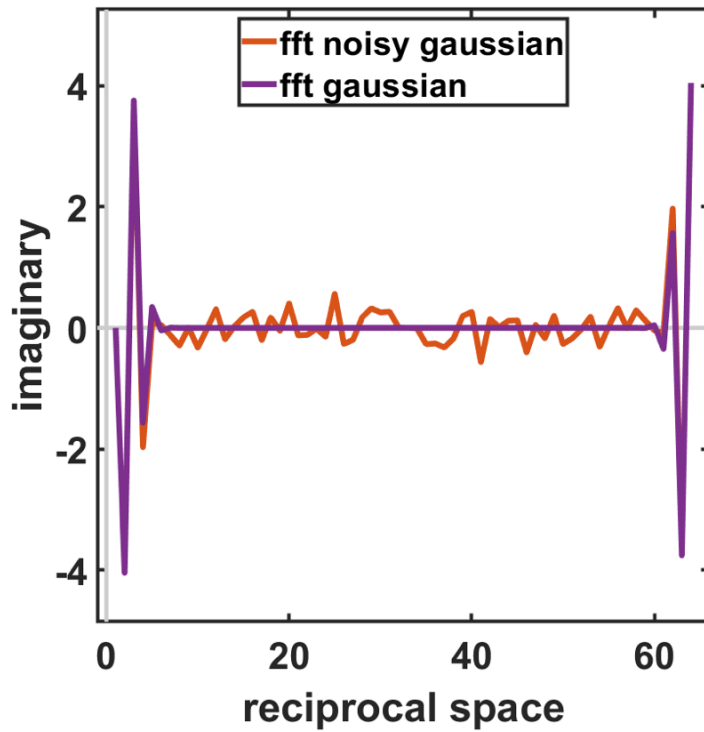


Figure 61. Imaginary parts of the DFTs of the broader, noise-free and noisy Gaussians in Figure 50 and Figure 57, respectively.

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 59 - Figure 61, 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 62 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
```

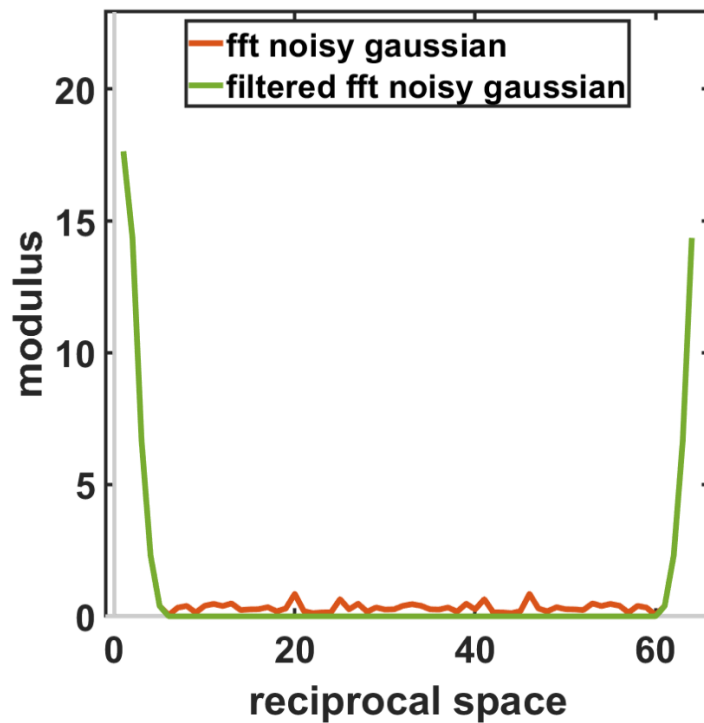


Figure 62. The modulus of the DFT of the noisy Gaussian plotted in Figure 57 and the same Fourier coefficients after those between positions 6 and 60 were zeroed out.

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 63, 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
```

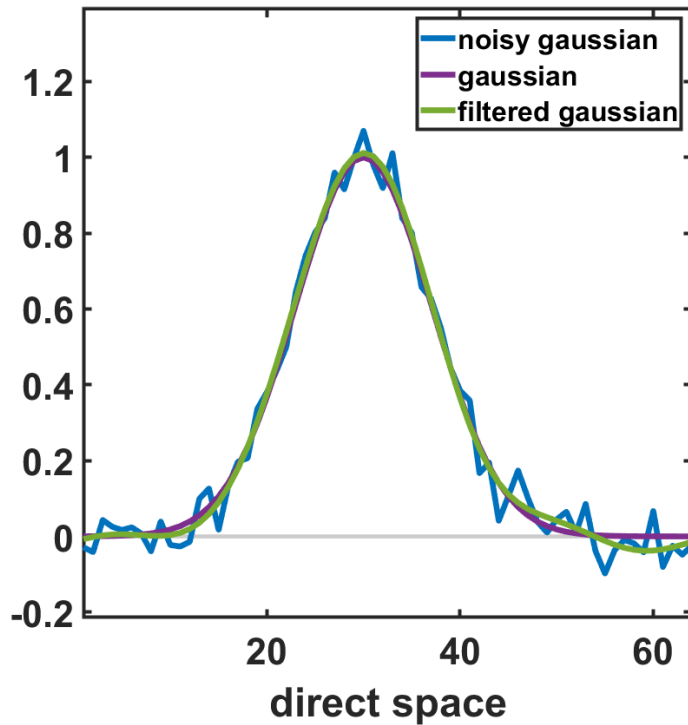


Figure 63. Overlay of the noise-free Gaussian in Figure 50, the noisy Gaussian produced from it in Figure 57, and the signal produced by denoising the noisy Gaussian in Figure 57.

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.

M. *Redundancy in the DFT*

The reader may have wondered why the DFTs in this section look different from the DFT in Figure 4. The reader may also have noticed that, just like the Fourier transform of a real function is Hermitian, the real parts of the DFTs in this section are even and their imaginary parts are odd. Furthermore, their moduli are even. Thus, there is a redundancy to the DFT as it is displayed in this section. Accordingly, a DFT can still be well represented by only displaying half of its

modulus, as in Figure 4. Technically speaking, this middle frequency is the Nyquist frequency. Above this frequency, no new information from the DFT is obtained.

N. *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:

$$DFT[x_i + y_i] = C_j + D_j \quad (250)$$

Furthermore, if a and b are constants:

$$DFT[ax_i + by_i] = aC_j + bD_j \quad (251)$$

We can prove Equation 251 by writing:

$$DFT[ax_i + by_i] \tag{252}$$

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

where the first result (in Equation 250) is proved by taking $a = b = 1$ in Equation 252.

2. First shifting theorem

Weaver refers to this theorem as the ‘first shifting theorem’.⁹ To prove it, first assume that x_i and its DFT, C_k , are sequences of length N . Now 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 226) in this derivation.

$$x_{n-s} = \sum_{k=0}^{N-1} C_k W_N^{(n-s)k} = \sum_{k=0}^{N-1} C_k W_N^{nk} W_N^{-sk} = \sum_{k=0}^{N-1} (C_k W_N^{-sk}) W_N^{nk} \tag{253}$$

That is, $x_{n-s} = DFT^{-1}(C_k W_N^{-sk})$, i.e., $DFT(x_{n-s}) = C_k W_N^{-sk}$. 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 $x_i e^{-i2\pi is/N}$, where s is a constant? We proceed as follows:

$$\begin{aligned} DFT(x_j e^{-i2\pi js/N}) &= \sum_{n=0}^{N-1} x_n e^{-i2\pi ns/N} e^{-i2\pi k(n/N)} \\ &= \sum_{n=0}^{N-1} x_i e^{-i2\pi(s+k)n/N} = C_{s+k} \end{aligned} \tag{254}$$

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

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: $DFT(x_j e^{-i2\pi js/N}) = C_{s+k}$. It follows that: $DFT(x_j e^{i2\pi js/N}) = C_{-s+k}$. Thus, we write out:

$$x_j e^{-i2\pi js/N} = x_j (\cos(2\pi js/N) - i \sin(2\pi js/N)) \quad (255)$$

$$x_j e^{i2\pi js/N} = x_j (\cos(2\pi js/N) + i \sin(2\pi js/N)) \quad (256)$$

Adding Equations 255 and 256 gives:

$$x_j e^{-i2\pi js/N} + x_j e^{i2\pi js/N} = 2x_j \cos(2\pi js/N) \quad (257)$$

Accordingly:

$$\begin{aligned} DFT(x_j e^{-i2\pi js/N}) + DFT(x_j e^{i2\pi js/N}) &= DFT(x_j e^{-i2\pi js/N} + x_j e^{i2\pi js/N}) \\ &= C_{s+k} + C_{-s+k} = DFT(2x_j \cos(2\pi js/N)) \end{aligned} \quad (258)$$

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

If instead of adding Equations 255 and 256 we subtract them, we obtain:

$$x_j e^{-i2\pi js/N} - x_j e^{i2\pi js/N} = -2ix_j \sin(2\pi js/N) \quad (259)$$

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 $DFT(DFT(x_j))$?

We proceed as follows:

$$\begin{aligned} DFT(DFT(x_j)) &= DFT(C_k) = \sum_{k=0}^{N-1} C_k e^{-i2\pi jk/N} = N \left(\frac{1}{N} \sum_{k=0}^{N-1} C_k e^{i2\pi(-j)k/N} \right) \\ &= Nx_{-j} \end{aligned} \quad (260)$$

This result is analogous to the result we obtained for the Fourier transform of the Fourier transform in Equation 129.

O. The two-dimensional (2D) DFT

1. Definition of the two-dimensional (2D) DFT

The DFT can be extended to two dimensions, which is particularly important in image processing. That is, for an image, a rectangular array, $x_{m,n}$, with $M \times N$ data points, we can write:

$$C_{k,l} = \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} x_{m,n} e^{-i2\pi k(n/N)} e^{-i2\pi l(m/M)} = \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} x_{m,n} e^{-i2\pi \left(\frac{kn}{N} + \frac{lm}{M} \right)} \quad (261)$$

$$x_{m,n} = \frac{1}{MN} \sum_{l=0}^{M-1} \sum_{k=0}^{N-1} C_{k,l} e^{i2\pi n(k/N)} e^{i2\pi m(l/M)} = \frac{1}{MN} \sum_{l=0}^{M-1} \sum_{k=0}^{N-1} C_{k,l} e^{i2\pi \left(\frac{nk}{N} + \frac{ml}{M}\right)} \quad (262)$$

The 2D-DFT is governed by a set of theorems that are analogous to those for the one-dimensional DFT.

2. Addition, Sum, or Linearity Theorem for the 2D-DFT

Consider two $M \times N$ rectangular arrays that we represent as $x_{m,n}$ and $y_{m,n}$, which have 2D-DFTs of $C_{k,l}$ and $D_{k,l}$. What is the 2D DFT of $a \cdot x_{m,n} + b \cdot y_{m,n}$, where a and b are constants? To obtain this result, we put $a \cdot x_{m,n} + b \cdot y_{m,n}$ into the definition for the 2D-DFT, as follows:

$$\begin{aligned} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} (a \cdot x_{m,n} + b \cdot y_{m,n}) e^{-i2\pi \left(\frac{kn}{N} + \frac{lm}{M}\right)} & \quad (263) \\ &= \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} a \cdot x_{m,n} e^{-i2\pi \left(\frac{kn}{N} + \frac{lm}{M}\right)} \\ &+ \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} b \cdot y_{m,n} e^{-i2\pi \left(\frac{kn}{N} + \frac{lm}{M}\right)} = a \cdot C_{k,l} + b \cdot D_{k,l} \end{aligned}$$

Even though this result is conceptually simple, it is very important.

3. Periodicity of the 2D-DFT

From Equation 261, we learned that $\text{2D-DFT}\{x_{m,n}\} = C_{k,l}$. Starting with this derivation, it can be shown that the 2D-DFT is periodic. That is, we now demonstrate the periodicity of the 2D-DFT by showing that $C_{k+N,l+M} = C_{k,l}$ as follows:

$$\begin{aligned}
C_{k+N,l+M} &= \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} x_{m,n} e^{-i2\pi(k+N)(n/N)} e^{-i2\pi(l+M)(m/M)} \\
&= \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} x_{m,n} e^{-i2\pi(kn/N+Nn/N)} e^{-i2\pi(lm/M+Mm/M)} \\
&= \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} x_{m,n} e^{-i2\pi(kn/N)} e^{-in2\pi} e^{-i2\pi(lm/M)} e^{-im2\pi} \\
&= \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} x_{m,n} e^{-i2\pi(kn/N)} e^{-i2\pi(lm/M)} = C_{k,l}
\end{aligned} \tag{264}$$

Conclusions

In conclusion, we have described the Fourier transform, the discrete Fourier transform, and their two-dimensional analogs. Both general mathematical principles related to these transforms and some of their theorems have been discussed. The Hilbert transform has also been described. As already noted, this tutorial does not cover every possible topic related to Fourier theory. Nevertheless, it should provide the interested reader with more information and knowledge, which should be helpful when denoising spectra. This tutorial contains quite a few figures that illustrate the concepts explained in it. Because of its ability to separate signal from noise in reciprocal space, Fourier theory provides an effective way to remove noise from spectra.

Statement of Attribution

This document was written by Linford. Gerashchenko made the excellent figures in it, where he understood the concepts behind these 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.

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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.

References

1. Lizarbe AJ, Wright KS, Lewis G, Murray G, Austin DE, Terry J, Aspnes DE, Linford MR, *Journal of Vacuum Science & Technology A* 43, 033401 (**2025**).
2. Savitzky A, Golay MJE, *Analytical Chemistry* 36, 1627–1639 (**1964**).
3. Bracewell RN, *The Fourier Transform and its Applications* (McGraw-Hill, **2000**)
4. Bracewell RN, *The Hartley Transform* (Oxford University Press, **1986**)
5. Smith J, *The Doctrine and Covenants of the Church of Jesus Christ of Latter-day Saints* (The Church of Jesus Christ of Latter-day Saints, Salt Lake City, Utah, USA, **1981**)
6. Körner TW, *Fourier Analysis* (Cambridge University Press, **1988**)
7. Kraniuskas P, *Transforms in Signals and Systems* (Addison-Wesley, **1992**)
8. Kraniuskas P, *IEEE Signal Processing Society* 11, 24–35 (**1994**).
9. Weaver HJ, *Theory of Discrete and Continuous Fourier Analysis* (John Wiley & Sons, **1989**)
10. Weaver HJ, *Applications of Discrete and Continuous Fourier Analysis* (John Wiley, **1983**)
11. Brigham EO, *The Fast Fourier Transform* (Prentice Hall, **1973**)
12. Walker JS, *Fast Fourier Transforms* (CRC Press, **1996**)
13. Konishi K, *Discrete Fourier Transform in Linear Algebra* **2025**)
14. Leis JW, *Digital Signal Processing Using MATLAB for Students and Researchers* (Wiley, **2011**)
15. Cartinhour J, *Digital Signal Processing An Overview of Basic Principles* (Prentice Hall, **2000**)
16. Lyons RG, *Understanding Digital Signal Processing* (Prentice Hall, **2011**)

17. Solomon C, Breckon T, *Fundamentals of Digital Image Processing A Practical Approach with Examples in MATLAB* (Wiley-Blackwell, **2011**)
18. Bagchi S, Mitra SK, *The Nonuniform Discrete Fourier Transform and Its Applications in Signal Processing* (Springer US, **1998**)
19. Amidror I, *Mastering the Discrete Fourier Transform in One, Two or Several Dimensions: Pitfalls and Artifacts* (Springer, **2013**)
20. Gaskill JD, *Linear Systems, Fourier Transforms, and Optics* (Wiley, **1978**)
21. Oppenheim AV, Schafer RW, Buck JR, *Discrete-Time Signal Processing* (Prentice Hall, New Jersey, **1989**)
22. Bracewell RN, *Fourier Analysis and Imaging* (Kluwer Academic/Plenum Publishers, New York, **2003**)
23. Lighthill MJ, *Fourier Analysis and Generalized Functions* (Cambridge University Press, **1970**)
24. Bloomfield P, *Fourier Analysis of Time Series* (John Wiley & Sons, **1976**)
25. Charles C, Leclerc G, Pireaux J-J, Rasson J-P, *Surface and Interface Analysis* 36, 49–60 (**2004**).
26. Charles C, Leclerc G, Rasson J-P, Pireaux J-J, *Surface and Interface Analysis* 36, 61–70 (**2004**).
27. Charles C, Leclerc G, Louette P, Rasson J-P, Pireaux J-J, *Surface and Interface Analysis* 36, 71–80 (**2004**).
28. Daubechies I, *Ten Lectures on Wavelets* (Society for Industrial and Applied Mathematics, , edition =, **1992**)
29. Moeini B, Avval TG, Gallagher N, Linford MR, *Surface and Interface Analysis* 55, 798–807 (**2023**).
30. Artyushkova K, Fulghum JE, *Surface and Interface Analysis* 33, 185–195 (**2002**).
31. Artyushkova K, Fulghum JE, *Surface and Interface Analysis* 36, 1304–1313 (**2004**).
32. Moeini B, Gallagher N, Linford MR, *Surface and Interface Analysis* 55, 853–858 (**2023**).
33. Moeini B, Linford JM, Gallagher N, Linford MR, *Surface and Interface Analysis* 56, 73–81 (**2024**).
34. Major GH, Fairley N, Fernandez V, Linford MR, *Vacuum Technology & Coating* 23(3), 34 (**2022**).
35. Le VL, Kim TJ, Kim YD, Aspnes DE, *Journal of Vacuum Science & Technology B* 37, 052903 (**2019**).
36. Le VL, Kim TJ, Kim YD, Aspnes DE, *Journal of the Korean Physical Society* 77, 819–823 (**2020**).
37. Le LV, Kim TJ, Kim YD, Aspnes DE, *Journal of the Korean Physical Society* 81, 403–408 (**2022**).
38. Blanchard P, Devaney RL, Hall GR, *Differential Equations* (Brooks/Cole CENGAGE Learning, **2012**)
39. Boas ML, *Mathematical Methods in the Physical Sciences, 2nd Edition* (Wiley, **1983**)
40. Arfken GB, Weber HJ, Harris F, *Mathematical Methods for Physicists, 5th Edition* (Academic Press, **2000**)
41. Gerashchenko M, Andersen T, konishi k, Aspnes DE, Linford M, *Vacuum Technology & Coating* 26(4), 27 (**2026**).

42. Lizarbe AJ, Wright KS, Austin DE, Aspnes DE, Linford MR, *Vacuum Technology & Coating* 24(7), 21 (**2024**).
43. Lizarbe AJ, Lewis G, Murray G, Wright KS, Austin DE, Aspnes DE, Linford MR, *Vacuum Technology & Coating* 24(8), 22 (**2024**).