The 1D Fourier Transform

The Fourier transform (FT) is important to the determination of molecular structures for both theoretical and practical reasons. On the theory side, it describes diffraction patterns and images that are obtained in the electron microscope. It is also the basis of 3D reconstruction algorithms. In the practical processing of EM images the FT is also useful because many operations, such as image filtering, are more easily and quickly done by the use of the transform and its inverse. We use the concepts of the FT so much in image processing and 3D reconstruction that having some acquaintance with the FT is essential to work in cryo-EM. You don't have to know how to do the integrals, but it is important to know the properties of the FT, for example what scaling or shifting of an image or volume does to the FT of that object. In what follows the important properties are highlighted thusly.

The Fourier transform (FT) converts one function into another. We write

$$g(x) \xrightarrow{FT} G(u)$$

where G is said to be the FT of g. It is obtained by multiplying the original function by a complex exponential and integrating:

$$G(u) = \int_{-\infty}^{\infty} g(x) e^{-i2\pi ux} dx \qquad (1)$$

The FT is a decomposition of a function into various frequency components. It maps a function in "real space" into "reciprocal space" or the "frequency domain". The inverse Fourier transform (IFT) takes us back to the original place:

$$g(x) = \int_{-\infty}^{\infty} G(u) e^{i2\pi ux} du. \qquad (2)$$

As you can see, the IFT is very similar to the FT, differing only in being the complex conjugate.

$$G(u) \xrightarrow{IFT} g(x).$$

Gaussian function

Let's take a specific choice for $g(x)$,

$$g(x) = e^{-\pi x^2}.$$

We can work out its FT by evaluating

$$\begin{aligned} G(u) &= \int_{-\infty}^{\infty} e^{-\pi x^2} e^{-i2\pi ux}\, dx \\ &= \int_{-\infty}^{\infty} e^{-\pi(x^2 + i2ux)}\, dx \end{aligned}$$

This integral can be evaluated by completing the square in the exponent,

$$G(u)=\int_{-\infty}^{\infty} e^{-\pi(x^2+i2ux-u^2)}dx\cdot e^{-\pi u^2}$$
$$=\int_{-\infty}^{\infty} e^{-\pi(x+iu)^2}dx\cdot e^{-\pi u^2}$$

It turns out that the integral itself in the last line is equal to 1. (This comes from the fact that the definite integral of $e^{-\pi x^2}$ is the same whether it's taken from $-\infty$ to ∞ or from $-\infty+iu$ to $\infty+iu$.)

The final result is that

$$G(u)=e^{-\pi u^2},$$

so in this special case, both the function and its Fourier transform are the same. This is in fact the only simple function for which this is true, and it can be summarized by

$$e^{-\pi x^2}\xrightarrow{FT}e^{-\pi u^2} \qquad (3)$$

(There is another function that is its own Fourier transform, but it's not so simple, as we'll see later.) What if we were to change the scaling of the Gaussian function? Let's make $g(x)$ narrower by the factor a, while preserving its area. The transform pair becomes

$$ae^{-\pi(ax)^2}\xrightarrow{FT}e^{-\pi(u/a)^2} \qquad (4)$$

the narrower function of x transforms into a *broader* function of u! Here's how it comes about. The FT of $ae^{-\pi(ax)^2}$ is

$$G(u)=\int_{-\infty}^{\infty} ae^{-\pi(ax)^2}e^{-i2\pi ux}\,dx\,.$$

Now we do a change of variables $y=ax$:

$$G(u)=\int_{-\infty}^{\infty} e^{-\pi y^2}e^{-i2\pi uy/a}\,dy$$
$$=e^{-\pi(u/a)^2}$$

Rect function

As one more specific example, consider the "rect function", which defines a rectangular pulse of unit area,

$$\mathrm{rect}(x)=\begin{cases}1, & |x|<1/2\\ 0, & \text{otherwise}\end{cases}$$

in this case the FT pair is[1]

[1] You can derive this too.

$$\mathrm{rect}(x) \xrightarrow{FT} \frac{\sin \pi u}{\pi u} \qquad (5)$$

the function on the right comes up very often, and it has a name, the "sinc" function:

$$\mathrm{sinc}(u) = \frac{\sin \pi u}{\pi u}.$$

The transform relationship goes in the opposite direction as well,

$$\mathrm{sinc}(x) \xrightarrow{FT} \mathrm{rect}(u). \qquad (6)$$

Please note that not everyone defines the sinc function the same way, so check to see that you're using the right one. I'm using the "normalized sinc function" that is popular in signal processing; mathematicians define $\mathrm{sinc}(x) = \sin x \,/\, x$.

Delta function

Finally, let's consider taking a very brief Gaussian pulse. We define the limiting form of this as the Dirac delta function,

$$\delta(x) = \lim_{a \to \infty} a e^{-\pi (ax)^2}$$

and obtain its Fourier transform by invoking eqn. (4) above. The result is

$$\delta(x) \xrightarrow{FT} 1 \qquad (7)$$

and

$$1 \xrightarrow{FT} \delta(u). \qquad (8)$$

The delta function has some special properties. The value of $\delta(x)$ is zero everywhere except when x=0; at that point its value is infinite. The integral of a delta function is equal to one, and the integral of a delta function times another function

$$\int_{-\infty}^{\infty} f(x)\delta(x-b)\,dx = f(b) \qquad (9)$$

$$\begin{aligned} G(u) &= \int_{-1/2}^{1/2} e^{-i2\pi ux}\,dx \\ &= \int_{-1/2}^{1/2} \cos(2\pi ux)\,dx \\ &= \frac{1}{2\pi u} \sin(2\pi ux)\Big|_{-1/2}^{1/2} \\ &= \frac{1}{\pi u} \sin(\pi u) \end{aligned}$$

is simply a value of the function, here *f*(*b*).

A really simple exercise. Use eqns. (9) and (1) to prove the Fourier transform relation (7).

Sampling

One more function to consider: a one-dimensional lattice. This is an infinite series of delta functions, spaced one unit apart. It is called the Dirac comb function or the shah function (the latter is named after the Russian letter Ш). Its transform is also a shah function.

$$\sum_{n=-\infty}^{\infty}\delta(x-n)\xrightarrow{FT}\sum_{m=-\infty}^{\infty}\delta(u-m) \qquad (10)$$

Properties of the 1D Fourier transform

Once you know a few transform pairs like the ones I outlined above, you can compute lots of FTs very simply using the following properties of transform pairs:

1. Linearity

$$g+h\xrightarrow{FT}G+H$$

2. Scale

$$g(ax)\xrightarrow{FT}\tfrac{1}{a}G\left(\tfrac{u}{a}\right)$$

3. Shift

$$g(x-b)\xrightarrow{FT}G(u)e^{-i2\pi ub}$$

4. Convolution

$$g*h\xrightarrow{FT}G\cdot H$$

The linearity property is pretty easy to understand, since the integral of a sum is the same as the sum of the integrals. We have mentioned the scale property already in eqn. (4), but an important use of the scale property has to do with the comb function (10). Its transform's spacing changes reciprocally when you change the comb's spacing,

$$\sum_{n=-\infty}^{\infty}\delta(ax-n)\xrightarrow{FT}\frac{1}{a}\sum_{m=-\infty}^{\infty}\delta\left(\frac{u}{a}-m\right) \qquad (11)$$

and as comb functions can be used to describe a crystal lattice, this reciprocal relationship gives rise to the term “reciprocal space” in crystallography.

The shift property can be proven in the following way. Let $f(x)=g(x-b)$. Then its FT is

$$F(u) = \int_{-\infty}^{\infty} g(x-b) e^{-i2\pi ux}\, dx$$

Now making the substitution $y=x-b$,

$$F(u) = \int_{-\infty}^{\infty} g(y) e^{-i2\pi u(y+b)}\, dy$$
$$= \int_{-\infty}^{\infty} g(y) e^{-i2\pi uy}\, dy \cdot e^{-i2\pi ub}$$
$$= G(u) e^{-i2\pi ub}.$$

Convolution

The final property, called convolution, is very important, so let me explain what it is. If we say that a function f is the convolution of g and h

$$f = g * h$$

we mean that f is given by

$$f(x) = \int_{-\infty}^{\infty} g(x-s) h(s)\, ds\,. \qquad (12)$$

That is, the value of $f(x)$ is given by values of g in the neighborhood of x, weighted by the values of h. Although it's not obvious at first glance, it turns out that convolution is commutative, that is $g * h = h * g$. (Try proving it!) The Fourier convolution property says that the FT of f is simply the product of the FTs of g and h.

Here is the proof. The FT of f is

$$F(u) = \iint g(x-s) h(s) e^{-i2\pi xu}\, ds\, dx$$
$$= \iint g(x-s) h(s) e^{-i2\pi (x-s)u} e^{-i2\pi su}\, ds\, dx$$

now, using the substitution $x' = x - s$ and exploiting the fact that all the integrals are from minus infinity to infinity, we have

$$F(u) = \iint g(x') h(s) e^{-i2\pi x'u} e^{-i2\pi su}\, ds\, dx'$$
$$= \int g(x') e^{-i2\pi x'u} dx' \int h(s) e^{-i2\pi su} ds$$
$$= G(u) \cdot H(u)$$

An example of a convolution operation is the blurring of an image by the point-spread function of a microscope or the filtering of a signal. For example g could be the signal that goes into a filter, and h is a function whose breadth determines how much smoothing occurs in the filter. Typically a filtering operation takes a lot of computation; but in the "frequency domain" the filtering operation is very easy because it's simply a multiplication.

Another example of convolution is when h is a delta function or series of delta functions. When $h(x) = \delta(x-b)$, $g * h = g(x-b)$, so it's just a shifted copy of g. If h is a comb function, the convolution with h will yield periodic copies of g.

Cosine function

Here is one more FT pair that we can derive using the shift and linearity properties. Suppose we let g be the sum of two delta functions,

$$g(x) = \frac{1}{2}\delta(x+1) + \frac{1}{2}\delta(x-1)$$

then making use of eqn. (7) and the shift property we have

$$G(u) = \tfrac{1}{2}e^{i2\pi u} + \tfrac{1}{2}e^{-i2\pi u} \qquad (13)$$

Recall that $e^{iy} = \cos y + i\sin y$ and that the sum of the two complex exponentials in (13) will cancel out the sine terms, leaving

$$G(u) = \cos(2\pi u)$$

and so we have the Fourier transform pair of the cosine function and a pair of delta functions:

$$\tfrac{1}{2}\delta(x+1) + \tfrac{1}{2}\delta(x-1) \xrightarrow{FT} \cos(2\pi u) \qquad (14)$$

Power Spectrum

Suppose you want to take the FT of a random signal. Its FT will also be random, but it can have a useful underlying structure. In the same way that the variance of a random variable gives information about the magnitude of that variable, the power spectrum gives an idea of what Fourier components are large and which are small. The power spectrum $S(u)$is the magnitude squared of the FT,

$$S(u) = |F(u)|^2.$$

If the random signal has been filtered by some filter function H such that $F = G \cdot H$, then the spectrum is given by

$$S(u) = |G(u)H(u)|^2$$

And if F and H are statistically independent, cross-terms vanish and the expectation value of the spectrum (i.e. what you would get if you average the spectrum over many instances of the random signal) is given by

$$\langle S(u)\rangle = |G(u)|^2|H(u)|^2 \qquad (15)$$

If the filter function H is, say, the CTF, then the resulting spectrum will resemble the square of the CTF. This is illustrated in the figure below.

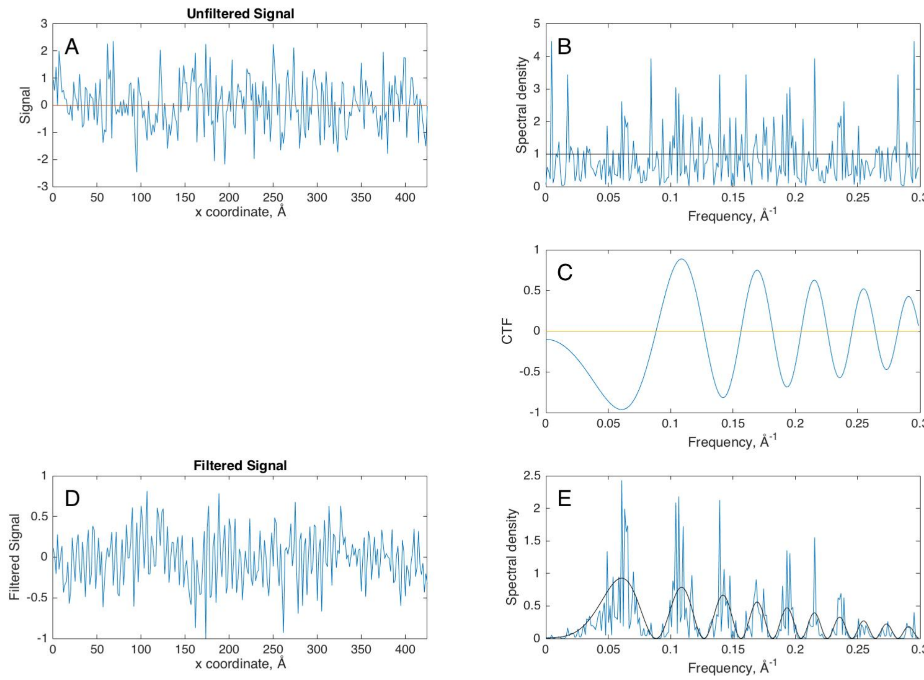

Figure 1. Power spectra of random signals. Left column, functions of *x*; right column, functions of the frequency variable *u*. A, the basic random signal, consisting of normally-distributed random numbers. B, its power spectrum. The mean value of the power spectrum is the same as the variance of the signal, 1 in this case. C, filter function—in this case, of the form of the defocus contrast-transfer function. D, the original signal, but with the CTF applied. E, power spectrum of the filtered signal, with a smooth curve superimposed, computed as $(CTF)^2$. Note that the power spectrum has minima at the same frequency values as zeros in the CTF.

Appendix

Correlation

An operation closely related to convolution is correlation, which is an operation that is often used to compare the similarity of two functions. If we say that $f(x)$ is the correlation $g \circ h$ we mean

$$f(x) = \int_{-\infty}^{\infty} g(x+s)h(s)ds. \qquad \text{(A1)}$$

This is the same as taking one function g, shifting it by x, and then multiplying it by another function h and summing the product up. If g and h are the same except that they're shifted relative to each other, then $f(x)$ will have a maximum at the proper shift value. The correlation has a simple Fourier transform too.

$$g \circ h \xrightarrow{FT} G \cdot H^*$$

where the asterisk means complex conjugate. This can be derived from the fact that reflection maps to complex conjugation, i.e.

$$g(-x) \xrightarrow{FT} G^*(u)$$

and the difference between the integrals in (12) and (A1) can be obtained if h is reflected.