

CHEM2024 - Week 22 Lecture 1 - Fourier transform

□ Chapter 15 of Steiner, "The Chemistry Maths Book", 2nd edition.

1. Definition and meaning

The *Fourier transform* is a connection between a signal recorded as a function of time (*time domain representation*) and the same signal recorded as a function of frequency (*frequency domain representation*).

Either representation defines the signal completely, we can freely move between them.

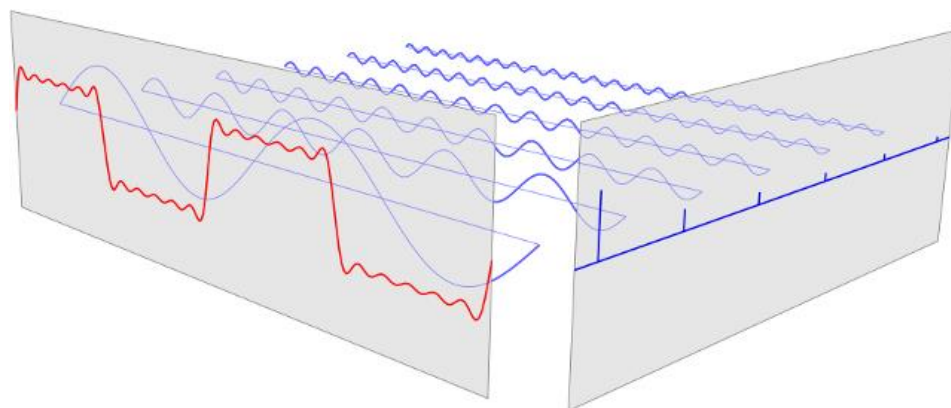


Figure 1. A schematic illustration of the decomposition of a function into a discrete sum of sines and cosines (source: Wikipedia). The Fourier transform is the continuous version of this procedure that also works for non-periodic functions.

This connection between the two representations $f(t)$ and $f(\omega)$ may be derived formally, but in this course we would simply state it without proof:

$$f(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt \quad f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(\omega) e^{+i\omega t} d\omega \quad (1)$$

The integral that produces $f(\omega)$ is called *forward Fourier transform*, and the integral that gives $f(t)$ back is called *backward Fourier transform*. Operator notation is often used:

$$\hat{F}_{\pm} f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{\mp i\omega t} dt \quad (2)$$

In situations when the time-dependent process $f(t)$ starts at time zero, the forward Fourier transform becomes *one-sided*:

$$\hat{F}_{+} f(t) = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} f(t) e^{-i\omega t} dt \quad (3)$$

The backward transform remains two-sided because negative frequencies may be present in $f(t)$. Definitions of Fourier transform in mathematics, physics, and engineering can differ in the location of the $\sqrt{2\pi}$ denominators; we use the *unitary definition* here.

Example 1: calculate the forward Fourier transform of a decaying oscillatory signal

$$f(t) = \begin{cases} e^{i\omega_0 t} e^{-kt} & t \geq 0 \\ 0 & t < 0 \end{cases}$$

Solution: the function is only non-zero for $t \geq 0$, the integration is therefore one-sided:

$$f(\omega) = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} e^{i\omega_0 t} e^{-kt} e^{-i\omega t} dt = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} e^{(i\omega_0 - k - i\omega)t} dt =$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{i(\omega_0 - \omega) - k} e^{(i\omega_0 - k - i\omega)t} \Big|_0^{\infty} = \frac{1}{\sqrt{2\pi}} \frac{1}{k + i(\omega - \omega_0)}$$

Separating real and imaginary components yields the Lorentz function (a peak at the frequency ω_0 in the real part of the Fourier transform:

$$f(\omega) = \frac{1}{\sqrt{2\pi}} \frac{1}{k + i(\omega - \omega_0)} = \frac{1}{\sqrt{2\pi}} \frac{k - i(\omega - \omega_0)}{k^2 + (\omega - \omega_0)^2} =$$

$$= \frac{1}{\sqrt{2\pi}} \frac{k}{k^2 + (\omega - \omega_0)^2} - \frac{i}{\sqrt{2\pi}} \frac{(\omega - \omega_0)}{k^2 + (\omega - \omega_0)^2}$$

This result – that each oscillatory component of the time domain signal corresponds to a peak in the frequency domain signal – is the foundation of digital signal processing.

2. Basic properties

Basic properties of forward and backward Fourier transforms are:

1. The two transforms are each other's inverse:

$$\hat{F}_- \hat{F}_+ f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} f(t') e^{i\omega t'} dt' \right] e^{-i\omega t} d\omega = f(t) \quad (4)$$

The proof is not straightforward, we shall skip it in this course.

2. Fourier transform is linear. For any two functions $f(t)$, $g(t)$ and for any two scalars α , β :

$$\hat{F}_{\pm} \{ \alpha f(t) + \beta g(t) \} = \alpha \hat{F}_{\pm} \{ f(t) \} + \beta \hat{F}_{\pm} \{ g(t) \} \quad (5)$$

The proof is obvious and relies on the linearity of the integration operation in Equations (1).

3. Fourier transform maps differentiation into multiplication. In the most common case (for chemical applications where time starts at zero) of the one-sided transform:

$$\hat{F}_+ \{ f'(t) \} = i\omega \hat{F}_+ \{ f(t) \} - f(0)/\sqrt{2\pi} \quad (6)$$

This is easy to prove using integration by parts:

$$\hat{F}_+ \{ f'(t) \} = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} f'(t) e^{-i\omega t} dt = \left\{ \begin{array}{ll} u = e^{-i\omega t} & du = -i\omega e^{-i\omega t} dt \\ dv = f'(t) dt & v = f(t) \end{array} \right\} =$$

$$= \frac{e^{-i\omega t} f(t)}{\sqrt{2\pi}} \Big|_0^{\infty} + \frac{i\omega}{\sqrt{2\pi}} \int_0^{\infty} f(t) e^{-i\omega t} dt = -\frac{f(0)}{\sqrt{2\pi}} + \frac{i\omega}{\sqrt{2\pi}} \int_0^{\infty} f(t) e^{-i\omega t} dt =$$

$$= i\omega \hat{F}_+ \{ f(t) \} - f(0)/\sqrt{2\pi}$$

Note that $f(0)$ refers to the original function of time, taken at time zero. This is particularly useful for solving differential equations, in which case $f(0)$ is the initial condition. Likewise, differentiation with respect to ω in the frequency domain is mapped into multiplication in the time domain:

$$\left[\hat{F}_{\pm} \{ f(t) \} \right]^{(k)} = (\mp i)^k \hat{F}_{\pm} \{ t^k f(t) \} \quad (8)$$

the simple proof is left as an exercise.

4. Fourier transform maps convolution into multiplication:

$$\begin{aligned} f * g &= \int_{-\infty}^{\infty} f(\tau) g(t-\tau) d\tau = \hat{F}_- \{ \hat{F}_+ \{ f(t) \} \hat{F}_+ \{ g(t) \} \} = \\ &= \hat{F}_+ \{ \hat{F}_- \{ f(t) \} \hat{F}_- \{ g(t) \} \} \end{aligned} \quad (9)$$

This is a very efficient way of applying convolution filters in digital signal processing. The proof is again laborious and will not be given in this course.

3. Applications

3.1 Differential equations

Property 3 from the previous section transforms many types of differential equations into algebraic equations. Consider a first order chemical kinetics process:

$$\frac{dA(t)}{dt} = -kA(t) \quad (10)$$

Taking the Fourier transform of both sides and using the property in Equation (7), we get:

$$\hat{F}_+ \left[\frac{dA(t)}{dt} \right] = -k \hat{F}_+ [A(t)] \Rightarrow i\omega A(\omega) - A_0 / \sqrt{2\pi} = -kA(\omega) \quad (11)$$

where A_0 is the initial concentration. The equation is now algebraic and therefore easy to solve:

$$A(\omega) = \frac{1}{\sqrt{2\pi}} \frac{A_0}{k + i\omega} \quad (12)$$

In practice, ordinary and partial differential equations are transformed into the frequency domain analytically and solved. The solutions are then numerically transformed back into the time domain.

Example 2: apply the one-sided Fourier transform to both sides of the following non-uniform ordinary differential equation using the initial condition $f(0) = 1$:

$$\frac{d}{dt} f(t) = -3f(t) + e^{-t}$$

Solution: the left hand side is exactly the same as in Equation (11)

$$\hat{F}_+ \left[\frac{d}{dt} f(t) \right] = i\omega f(\omega) - f(0) / \sqrt{2\pi} = i\omega f(\omega) - 1 / \sqrt{2\pi}$$

The right hand side requires some work:

$$\begin{aligned} \frac{1}{\sqrt{2\pi}} \int_0^{\infty} (-3f(t) + e^{-t}) e^{-i\omega t} dt &= -3f(\omega) + \frac{1}{\sqrt{2\pi}} \int_0^{\infty} e^{-(i\omega+1)t} dt = \\ &= -3f(\omega) + \frac{1}{\sqrt{2\pi}} \frac{1}{i\omega+1} \end{aligned}$$

Therefore, the resulting algebraic equation is:

$$i\omega f(\omega) - 1/\sqrt{2\pi} = -3f(\omega) + \frac{1}{\sqrt{2\pi}} \frac{1}{i\omega + 1}$$

3.2 Digital filters

Noise is often a problem in experimental data, but the frequencies expected in the signal may be different from the frequencies of the noise. This may be used to “clean up” the signal; the procedure is called *digital filtering*. As a simple example, the following transformation performs a forward Fourier transform, multiplies the unwanted frequencies by zero and performs a backward Fourier transform:

$$f(t) \leftarrow \hat{F}_- \left\{ M(\omega) \hat{F}_+ \{ f(t) \} \right\}, \quad M(\omega) = \begin{cases} 0 & \text{for unwanted } \omega \\ 1 & \text{for wanted } \omega \end{cases} \quad (13)$$

This transformation called a *bandpass filter* – it only keeps the frequencies that fall into the user-specified band. The selection function $M(\omega)$ is called *magnitude transfer function*. Similar transformations may be designed to shift, amplify and otherwise modify signal frequencies.

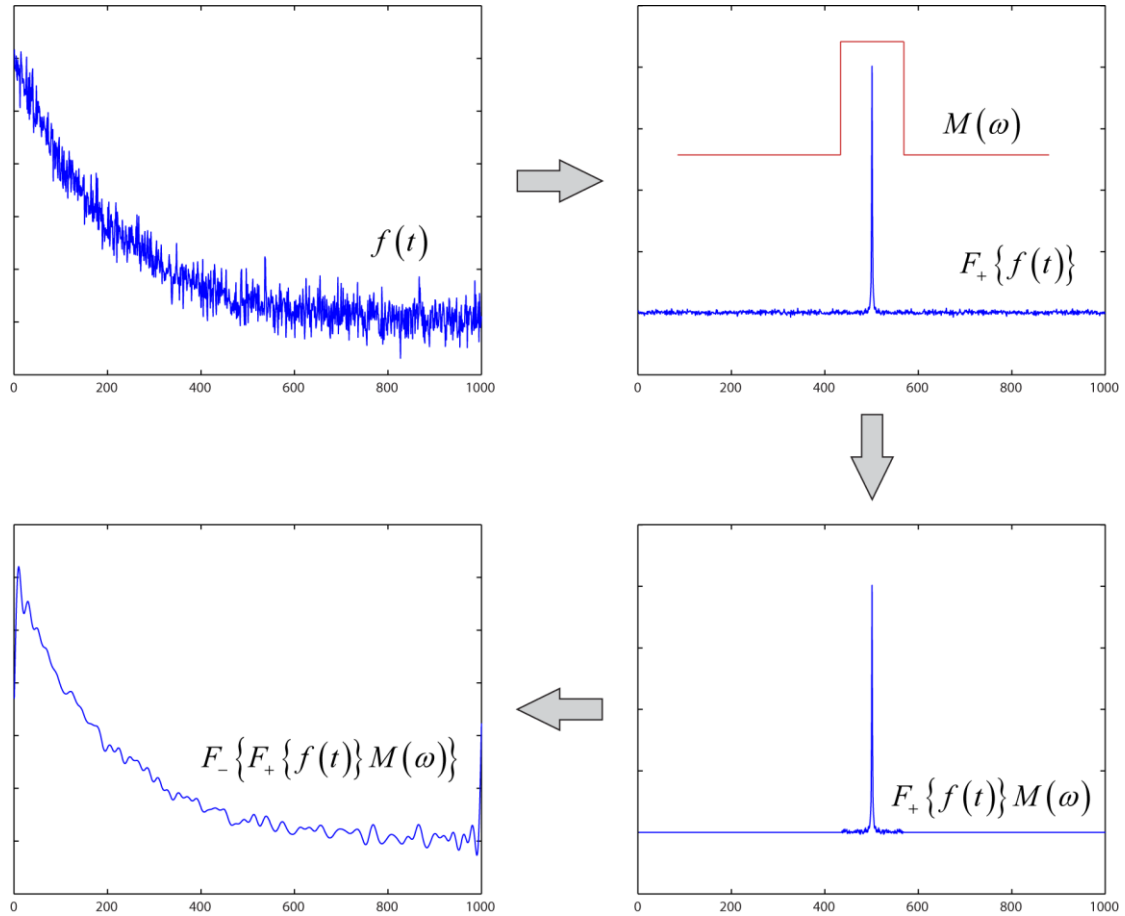


Figure 2. A bandpass filter applied to a noisy optical absorption signal of a decomposing chemical substance.

3.3 Image compression

In its most basic form, the JPEG image compression process first separates the image into luminance and chrominance channels. This is done because human eye is more sensitive to pixel brightness than colour. Each channel is then split into blocks of 16×16 pixels, and the blocks are Fourier transformed. All frequencies above a user-specified thresholds are zeroed out and the image stored as a table of the remaining non-zero coefficients, resulting in a significant reduction in the file size.



Figure 3. Blocking and high frequency information loss at high levels of JPEG compression.

When a JPEG file is opened, the reverse transformation is performed and the image is displayed. Some information is lost in the compression process, but the human eye is often unable to tell the difference. Typical JPEG artefacts are shown in Figure 3. Because high frequency information is discarded, JPEG works best on images containing smooth colour gradients.

4. Discrete and ‘fast’ Fourier transform

For discrete data, the integral in Equations (1) is replaced by the corresponding Riemann sum:

$$f(\omega_n) = \frac{1}{\sqrt{2\pi}} \sum_{k=0}^{N-1} f(t_k) e^{-i\omega_n t_k} \Delta t_k \quad (14)$$

where N is the total number of digitisation points in the signal, and the points are assumed to be uniformly spaced. The sum in Equation (14) has to be computed for every point in the spectrum, meaning that $O(N^2)$ multiplications are required for a size N Fourier transform. This makes brute-force evaluation slow. For the special case of $N = 2^n$, where n is a small integer, the Fourier transform can be broken down into smaller chunks, yielding $O(N \log_2 N)$ scaling, which is much better. This is called *fast Fourier transform*, it is used in most software packages these days.