Appendix A

Fourier transforms

A.1 Discrete FT

Consider a discrete periodic time series f_j, with period n. It is often useful to express such a time series as a sum over a set of n periodic functions $\exp(2\pi ikj/n)$, with k ranging from zero to $n-1$. We write

$$f_j = \sum_k \tilde{f}_k \exp(2\pi ikj/n) \tag{A.1.1}$$

We would like to extract the amplitude $\tilde{f}_k$, by an appropriate sum over the series f_j, making use of the orthogonality of the complex exponentials:

$$\tilde{f}_k = \frac{1}{n}\sum_j \exp(-2\pi ikj/n) f_j \tag{A.1.2}$$

To prove this relation, substitute the expansion for f_j into the above equation and reverse the order of summation:

$$\frac{1}{n}\sum_j \exp(-2\pi ikj/n) f_j = \sum_m \frac{1}{n}\sum_j \exp(2\pi i(m-k)j/n) \tag{A.1.3}$$

Consider the inner sum, which can be written in terms of the function

$$S_q = \frac{1}{n}\sum_{j=0}^{n-1} \exp(2\pi iqj/n) \tag{A.1.4}$$

with argument $q = m - k$. For nonzero q, we shall show that S_q vanishes.

To see this, note that the summands are the qth powers of the n complex nth roots of unity, which are uniformly spaced about the unit circle. Therefore, the summation index is periodic, and can be shifted by a constant without changing the sum. If we shift j by 1, we can show $S_q = \exp(2\pi iq/n)S_q$. Thus S_q equals zero unless $q = 0$, in which case $S_0 = 1$.

This result demonstrates the orthogonality of the complex exponential basis functions:

$$\frac{1}{n}\sum_j \exp(2\pi imj/n)\exp(-2\pi ikj/n) = \delta_{mk} \tag{A.1.5}$$

It also proves the completeness relation, by which we can represent the Kronecker delta as a sum over basis functions:

$$\frac{1}{n}\sum_j \exp(2\pi ikj/n) = \delta_{k0} \tag{A.1.6}$$

A.2 Fourier series

Consider a periodic continuous time series $f(x)$ with period L. We would like to represent this time series as a sum over the infinite set of complex exponentials $\exp(iqx)$, in which $q = 2\pi n/L$, and n ranges over the integers. We write

$$f(x) = \sum_q \tilde{f}_q \exp(iqx) \tag{A.2.1}$$

We wish to extract the Fourier amplitude f_q by again taking the inner product of $\exp(iqx)$ with $f(x)$:

$$\tilde{f}_q = 1/L \int_0^L dx\, \exp(-iqx) f(x) \tag{A.2.2}$$

As before, to prove that this relation holds, substitute the expansion for $f(x)$ on the right hand side, and reverse the order of summation and integration; we have

$$1/L \int_0^L dx\, \exp(-iqx) f(x) = \sum_{q'} f_{q'} (1/L) \int dx\, \exp(i(q'-q)x) \tag{A.2.3}$$

The integral is elementary,

$$(1/L) \int dx\, \exp(i(q'-q)x) = \delta qq' \tag{A.2.4}$$

which expresses the orthogonality of the complex basis functions, and proves the formula for the Fourier amplitude. It also proves the completeness relation

$$(1/L) \int dx\, \exp(iqx) = \delta_{q0} \tag{A.2.5}$$

A.3 Fourier transform

As the width of the domain $x = (0, L)$ (or equivalently $-L/2$ to $L/2$) increases, the discrete infinite set of wavenumbers grows more closely spaced. To take the limit of large L, we need to redefine the Fourier amplitudes in such a way as to eliminate explicit appearance of L, and create the necessary factors to turn $\sum_q$ into an integral.

Hence we rewrite $\tilde{f}_q$ as $1/L\tilde{f}(q)$, define $\Delta q = 2\pi/L$, and therefore write

$$\begin{aligned} f(x) &= 1/2\pi \int dq\, \tilde{f}(q) \exp(iqx) \\ \tilde{f}(q) &= \int dx\, \exp(-iqx) f(x) \\ 1/2\pi \int dx\, \exp(iqx) &= \delta(q) \end{aligned} \tag{A.3.1}$$

In the last expression, we have defined the delta-function $\delta(q)$ as the limit of $(L/2\pi)\delta_{q0}$. This is a narrow function, normalized in that

$$\int dq\, \delta(q) = \sum_q (2\pi/L)(L/2\pi)\delta_{q0} = 1 \tag{A.3.2}$$

The last of the above array of equations expresses the orthogonality of the complex exponential on the infinite interval, as well as the completeness relation (expansion of the delta function in basis functions).

A.4 Convolution theorem

Appendix B

Gaussians

B.1 Moment integrals

We begin with the integral of a Gaussian,

$$I_0(\alpha) = \int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} = (\pi/\alpha)^{1/2}$$

This result can be obtained by squaring I_0, interpreting the result as an integral over the x-y plane, and converting to polar coordinates:

$$I_0^2 = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\, e^{-\alpha(x^2+y^2)} \tag{B.1.1}$$

$$= \int_0^{\infty} rdr \int_0^{2\pi} d\theta\, e^{-\alpha r^2} \tag{B.1.2}$$

Now a change of variable $z = \alpha r^2$ gives $dz = 2\alpha r dr$, with the entire factor rdr now downstairs (which was the point of squaring I_0), so that we can perform the integral over r (giving a factor $1/(2\alpha)$ and θ (giving a factor 2π), leading to the result above.

To compute averages of powers of x in a Gaussian distribution, we require integrals of x^n times a Gaussian. If n is odd, the integral $\int_{-\infty}^{\infty} x^n e^{-\alpha x^2}$ vanishes by symmetry (integrand is odd). If n is even, we can generate the factor of x^n by taking successive derivatives of I_0 with respect to α. Each derivative brings down a factor of $-x^2$. Hence we have

$$\int_{-\infty}^{\infty} dx\, x^{2k} e^{-\alpha x^2} = (-\partial/\partial\alpha)^k I_0(\alpha)$$

For example,

$$\int_{-\infty}^{\infty} dx\, x^2 e^{-\alpha x^2} = (-\partial/\partial\alpha) I_0(\alpha) = \frac{\pi^{1/2}}{2\alpha^{3/2}} = \frac{I_0(\alpha)}{2\alpha}$$

We often require integrals in which a Gaussian integrand is multiplied by a simple exponential, as in

$$J = \int_{-\infty}^{\infty} dx\, e^{-\beta x} e^{-\alpha x^2} \tag{B.1.3}$$

One example of this form is the Fourier transform of a Gaussian of width σ,

$$I = \int_{-\infty}^{\infty} dx\, e^{-iqx} e^{-x^2/(2\sigma^2)} \tag{B.1.4}$$

Integrals like J can be evaluated by "completing the square" in the exponent, i.e., by writing the exponent as

$$\beta x + \alpha x^2 = \alpha(x - \beta/(2\alpha))^2 - \beta^2/(4\alpha) \tag{B.1.5}$$

Then we can shift the integration variable, defining $y = x - \beta/(2\alpha)$, so that

$$J = \int_{-\infty}^{\infty} dy\, e^{-\alpha y^2} e^{-\beta^2/(4\alpha)} = I_0(\alpha) e^{-\beta^2/(4\alpha)} \tag{B.1.6}$$

Using this result we have for the Fourier transform of a Gaussian of width σ, (with $\beta = iq$ and $\alpha = 1/(2\sigma^2)$),

$$I = \int_{-\infty}^{\infty} dx\, e^{-iqx} e^{-x^2/(2\sigma^2)} = I_0(1/(2\sigma^2)) e^{-q^2\sigma^2/2} \tag{B.1.7}$$

Note that the width of the Fourier transformed Gaussian is $1/\sigma$; a narrow Gaussian in "real space" transforms to a wide Gaussian in "reciprocal space", and vice versa.

B.2 Delta function

The simplest way to define a delta function is in terms of a limit of a narrow, conveniently integrated, normalized function:

$$\delta(t) = \lim_{\sigma \to 0} \frac{e^{-t^2/(2\sigma^2)}}{\sqrt{2\pi\sigma^2}} \tag{B.2.1}$$

Taking the Fourier transform of this definition,

$$\int dt e^{i\omega t} \frac{e^{-t^2/(2\sigma^2)}}{\sqrt{2\pi\sigma^2}} = e^{-\omega^2\sigma^2/2} \tag{B.2.2}$$

which in the limit $\sigma \to 0$ gives simply unity.

Inverting this Fourier transform, we have

$$\int d\omega 2\pi e^{-i\omega t} = \delta(t) \tag{B.2.3}$$

which is a useful integral representation of the delta function.