1 Spectral analysis

Astronomically forced phenomena such as glacial cycles give rise to signals in which periodic phenomena are superimposed on other types of variations.

One often seeks to measure the frequency of the various periodic components along with their relative amplitude.

To do so, we compute *power spectra*, using *Fourier transforms*.

These lectures are intended to provide a theoretical understanding of power spectra.

But we first consider some typical data.

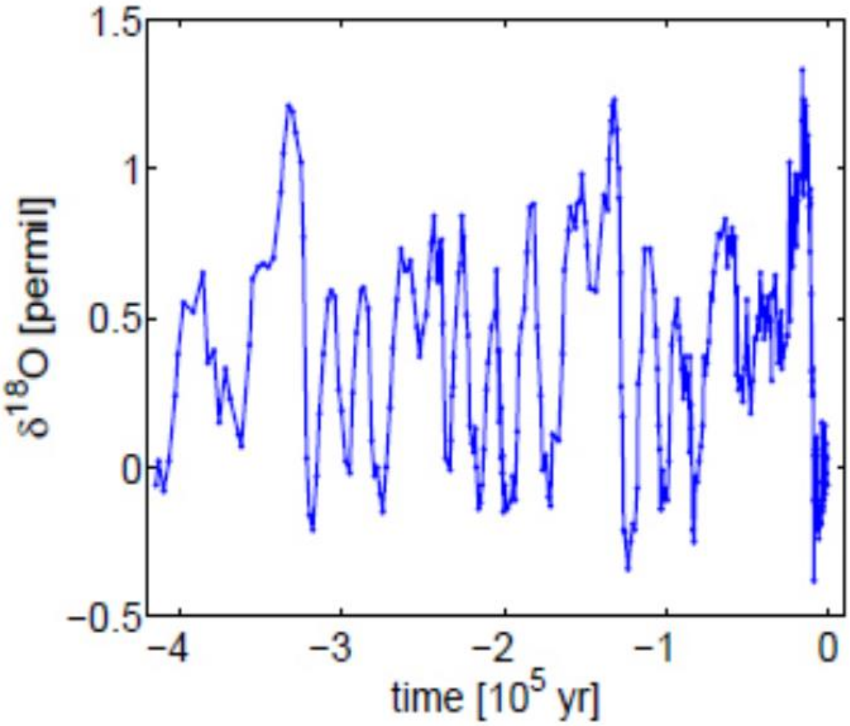
1.1 Climatic signals

Ocean sediments and ice cores contain within them a great many signals of climate change, e.g.

- Isotopic composition of oxygen, which is sensitive to global ice volume and temperature, obtained from
  - entrapped air in ice cores; and
  - carbonate shells of planktic (sea surface) and benthic (sea bottom) organisms.
- Deuterium/hydrogen ratios (D/H), $D = {}^2H$ (${}^1H$ with a neutron), sensitive to temperature, in ice cores.
- Carbon isotopic compositions.
- Dust content, etc.

Perhaps the most studied signal is

$$\delta^{18}O = \left(\frac{\left({}^{18}O/{}^{16}O\right)_{\text{sample}}}{\left({}^{18}O/{}^{16}O\right)_{\text{std}}} - 1 \right) \times 1000$$



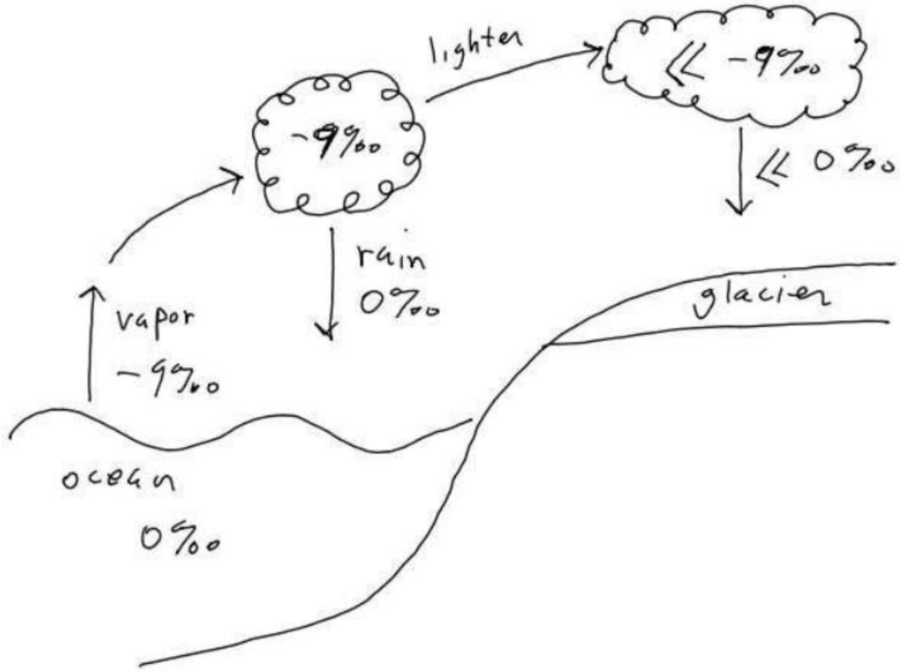
Note the clear occurrence of the precession signal, with a period of about 23 Kyr.

Many processes cause $\delta^{18}O$ to change. The two most important are the following:

- The vapor pressure (related to evaporation rate) of water containing ^{16}O is higher than that of water containing ^{18}O. Thus ^{16}O evaporates more readily, and *evaporated water is depleted in* ^{18}O.
- Conversely, *precipitated water is enriched in* ^{18}O. In other words, $H_2{}^{18}O$ condenses at a faster rate than $H_2{}^{16}O$.

The combined effect of these two processes leads to an enrichment of $\delta^{18}O$ of air as the global volume of ice grows.

Here's why:



Take ocean water to be at 0‰.

Evaporated water is typically about 9‰ lighter (at 20 °C) than liquid water.

Conversely condensate is about 9‰ heavier than vapor.

So a cloud forming from recently evaporated seawater has $\delta_{\text{cloud}} = -9‰$.

And the first rain from this cloud is 9‰ is heavier, so that $\delta_{\text{rain}} = 0‰$.

However the remaining water in the cloud must be isotopically lighter than it was originally, and the rain out of it will therefore also become lighter.

As the cloud moves to higher elevations or higher latitudes, it loses more vapor to condensate, and the resulting rain or snow becomes lighter and lighter.

This process, in which a particular mass—here a cloud—is progressively "milked" of the heavy isotope so that it becomes lighter and lighter (or vice-versa), is an example of *Rayleigh distillation*.

In the arctic, both clouds and the resulting snow are very light, less than

$-30‰$. The isotopic composition of the entire pool of condensate, from beginning to end, is of course equal to the original $-9‰$—but since the initial (low-latitude) precipitation is heavier, the final (high-latitude) precipitation must be much lighter.

Polar ice turns out to be about $-40‰$, i.e., about 4% lighter than the O_2 of seawater.

We also know that sea level was about 100 m lower during times of peak glaciation.

Since the average depth of the oceans is about 3800 m,

$$\frac{\text{total ice volume}}{\text{ice + ocean volume}} = \frac{100}{3800} = 2.6\%$$

Conservation of mass then requires that the isotopic composition δ_w of the remaining seawater satisfy

$$\frac{1}{38}(-40‰) + \frac{37}{38}\delta_w = 0$$

implying that

$$\delta_w \simeq 1.1‰.$$

The O_2 in the atmosphere is created by photosynthesis, from water:

$$CO_2 + H_2O \rightarrow CH_20 + O_2.$$

The $\delta^{18}O$ of entrapped air in ice cores should therefore change more or less as the $\delta^{18}O$ of seawater, i.e., it should be about $1‰$ heavier in glacial times than interglacials, just as seen in the Vostok ice core.

1.2 Fourier transforms

The precise oscillatory nature of an observed time series $x(t)$ is usually not identifiable from $x(t)$ alone.

We may ask

- How well-defined is the the dominant frequency of oscillation?
- How many frequencies of oscillation are present?
- What are the relative contributions of all frequencies?

The analytic tool for answering these and myriad related questions is the *Fourier transform.*

1.2.1 Continuous Fourier transform

We first state the Fourier transform for functions that are continuous with time.

The Fourier transform of a function $f(t)$ is

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

Similarly, the inverse Fourier transform is

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\omega) e^{i\omega t} \mathrm{d}\omega.$$

That the second relation is the inverse of the first may be proven, but we save that calculation for the discrete transform, below.

1.2.2 Discrete-time signals

We are interested in the analysis of observational or experimental data, which is almost always discrete. Thus we specialize to *discrete Fourier transforms.*

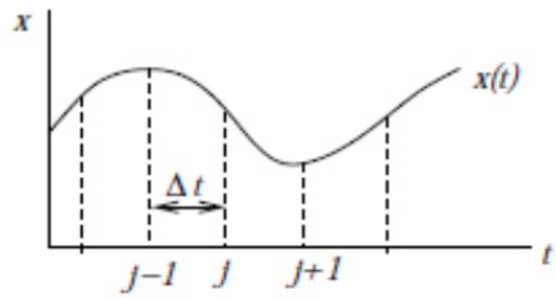
In modern data, one almost always observes a discretized signal

$$x_j, \qquad j = \{0, 1, 2, \ldots, n-1\}$$

We take the *sampling interval*—the time between samples—to be Δt. Then

$$x_j = x(j\Delta t).$$

The discretization process is pictured as

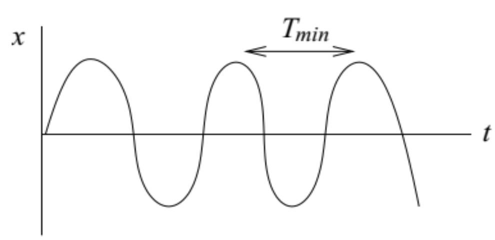


A practical question concerns the choice of Δt. To choose it, we must know the highest frequency, f_{max}, contained in $x(t)$.

The shortest period of oscillation is

$$T_{\mathrm{min}} = 1/f_{\mathrm{max}}$$

Pictorially,



We require at least two samples per period. Therefore

$$\Delta t \leq \frac{T_{\mathrm{min}}}{2} = \frac{1}{2f_{\mathrm{max}}}.$$

To see why, we note that if a continuous signal $f(t)$ contains no frequencies greater than f_{max}, the inverse Fourier transform of $F(\omega)$ may be written

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-2\pi f_{\mathrm{max}}}^{2\pi f_{\mathrm{max}}} F(\omega) e^{i\omega t} \mathrm{d}\omega$$

since $F(\omega) = 0$ when $|\omega| > 2\pi f_{\mathrm{max}}$.

Now define the jth sampling time

$$t_j = j\frac{T_{\min}}{2} = \frac{j}{2f_{\max}}, \qquad j = \ldots -1, 0, 1 \ldots$$

Substituting t_j for t above, we obtain

$$f(t_j) = \frac{1}{\sqrt{2\pi}} \int_{-2\pi f_{\max}}^{2\pi f_{\max}} F(\omega) e^{i\omega t_j} \mathrm{d}\omega.$$

The RHS is the jth coefficient in a Fourier-series expansion of $F(\omega)$.

Consequently the sampled function $f(t_j)$ completely determines $F(\omega)$.

And by inverse Fourier transformation, the continuous function $f(t)$ is completely determined by $F(\omega)$.

This reasoning, first given by Shannon [6], leaves open the question of how to reconstruct the continuous function $f(t)$ when only $f(t_j)$ is known.

In principle, exact interpolation is possible via the convolutional sum

$$f(t) = \sum_{j=-\infty}^{\infty} x_j \frac{\sin \pi(2f_{\max}t - j)}{\pi(2f_{\max}t - j)}.$$

where $x_j = f(t_j)$.

1.2.3 Discrete Fourier transform

The discrete Fourier transform (DFT) of a time series $x_j, j = 0, 1, \ldots, n-1$ is

$$\hat{x}_k = \sum_{j=0}^{n-1} x_j \exp\left(-i\frac{2\pi jk}{n}\right) \qquad k = 0, 1, \ldots, n-1$$

To gain some intuitive understanding, consider the range of the exponential multiplier.

- $k = 0 \Rightarrow \exp(-i2\pi jk/n) = 1$. Then

$$\hat{x}_0 = \sum_j x_j$$

Thus $\hat{x}_0$ is n times the mean of the x_j's.

This is the "DC" component of the transform.

Question: Suppose a seismometer measures ground motion. What would $\hat{x}_0 \neq 0$ mean?

- $k = n/2 \Rightarrow \exp(-i2\pi jk/n) = \exp(-i\pi j)$. Then

$$\begin{aligned} \hat{x}_{n/2} &= \sum_j x_j(-1)^j \\ &= x_0 - x_1 + x_2 - x_3 \dots \end{aligned}$$

  Frequency index $n/2$ is clearly the highest accessible frequency.

- The frequency indices $k = 0, 1, \dots, n/2$ correspond to frequencies

$$f_k = k/t_{\max},$$

  i.e., k oscillations per $t_{\max}$, the period of observation.
  Index $k = n/2$ then corresponds to

$$f_{\max} = \left(\frac{n}{2}\right)\left(\frac{1}{n\Delta t}\right) = \frac{1}{2\Delta t}$$

But if $n/2$ is the highest frequency that the signal can carry, what is the significance of $\hat{x}_k$ for $k > n/2$?

For real x_j, frequency indicies $k > n/2$ are *redundant*, being related by

$$\hat{x}_k = \hat{x}^*_{n-k}$$

where z^* is the complex conjugate of z (i.e., if $z = a + ib$, $z^* = a - ib$).

We derive this relation as follows. From the definition of the DFT, we have

$$\begin{aligned}\hat{x}^*_{n-k} &= \sum_{j=0}^{n-1} x_j \exp\left(+i\frac{2\pi j(n-k)}{n}\right) \\ &= \sum_{j=0}^{n-1} x_j \underbrace{\exp\left(i2\pi j\right)}_{1} \exp\left(\frac{-i2\pi jk}{n}\right) \\ &= \sum_{j=0}^{n-1} x_j \exp\left(\frac{-i2\pi jk}{n}\right) \\ &= \hat{x}_k\end{aligned}$$

where the + in the first equation derives from the complex conjugation, and the last line again employs the definition of the DFT.

Note that we also have the relation

$$\hat{x}^*_{-k} = \hat{x}^*_{n-k} = \hat{x}_k.$$

The frequency indicies $k > n/2$ are therefore sometimes referred to as *negative frequencies*

1.2.4 Inverse discrete Fourier tranform

The inverse DFT is given by

$$x_j = \frac{1}{n}\sum_{k=0}^{n-1} \hat{x}_k \exp\left(+i\frac{2\pi jk}{n}\right) \qquad j = 0, 1, \ldots, n-1$$

We proceed to demonstrate this inverse relation.

We begin by substituting the DFT for $\hat{x}_k$, using dummy variable j':

$$\begin{aligned} x_j &= \frac{1}{n}\sum_{k=0}^{n-1}\left[\sum_{j'=0}^{n-1} x_{j'} \exp\left(-i\frac{2\pi j'k}{n}\right)\right] \exp\left(+i\frac{2\pi kj}{n}\right) \\ &= \frac{1}{n}\sum_{j'=0}^{n-1} x_{j'} \sum_{k=0}^{n-1} \exp\left(-i\frac{2\pi k(j'-j)}{n}\right) \\ &= \frac{1}{n}\sum_{j'=0}^{n-1} x_{j'} \times \begin{cases} n, & j' = j \\ 0, & j' \neq j \end{cases} \\ &= \frac{1}{n}(nx_j) \\ &= x_j \end{aligned}$$

The third relation derives from the fact that the previous $\sum_k$ amounts to a vanishing sum over the unit circle in the complex plane, except when $j' = j$.

To see why the sum over the circle vanishes, consider the example of

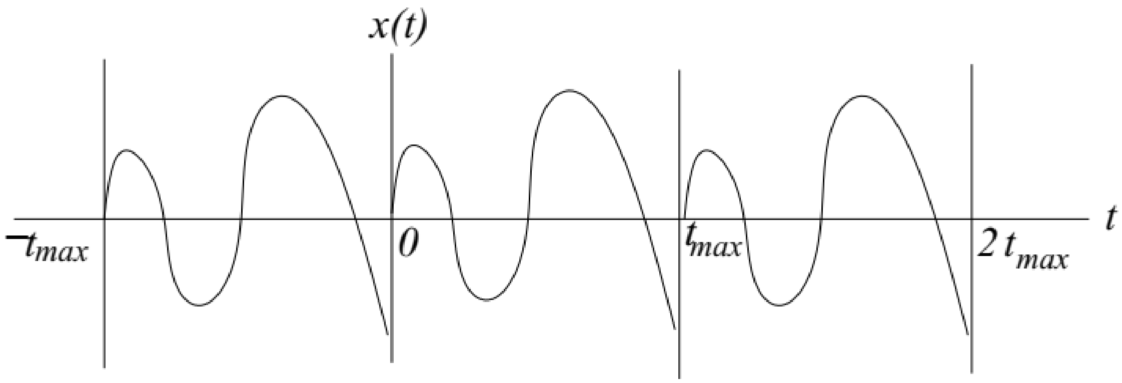
$$j' - j = 1 \quad \text{and} \quad n = 4.$$

The elements of the sum are then just the four points on the unit circle that intersect the real and imaginary axes, i.e.,

$$\begin{aligned} \sum_{k=0}^{3} \exp\left(-i\frac{2\pi k(j'-j)}{4}\right) &= e^0 + e^{-i\pi/2} + e^{-i\pi} + e^{-i3\pi/2} \\ &= 1 + i - 1 - i \\ &= 0. \end{aligned}$$

Finally, note that the DFT relations imply that x_j is periodic in n, so that $x_{j+n} = x_j$.

Consequently a finite time series is treated as if it were recurring:



1.3 The autocorrelation function and the power spectrum

Assume that the time series x_j has zero mean and that it is periodic, i.e., $x_{j+n} = x_j$.

Define the *autocorrelation function* ψ:

$$\psi_m = \sum_{j=0}^{n-1} x_j^* x_{j+m}$$

where

$$\psi_m = \psi(m\Delta t)$$

The autocorrelation function measures the degree to which a signal resembles itself over time. Thus it measures the predictability of the future from the past.

To gain some intuition:

- Consider, for example, $m = 0$ and real x_j. Then

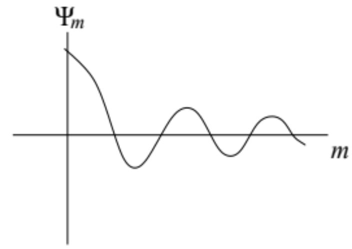
  $$\psi_0 = \sum_{j=0}^{n-1} x_j^2,$$

  which is n times the mean squared value of x_j.

- Alternatively, if $m\Delta t$ is much less than the dominant period of the data, ψ_m should not be too much less than ψ_0.

- Last, if $m\Delta_t$ is much greater than the dominant period of the data, $|\psi_m|$ is relatively small.

A typical ψ_m looks like



The *power spectrum* of a time series is the magnitude squared of its Fourier transform:

$$|\hat{x}_k|^2 = \left| \sum_{j=0}^{n-1} x_j \exp\left(-i\frac{2\pi jk}{n}\right) \right|^2 .$$

The *Wiener-Khintchin theorem* states that

power spectrum = Fourier transform of the autocorrelation.

In symbols,

$$|\hat{x}_k|^2 = \sum_{m=0}^{n-1} \psi_m \exp\left(-i\frac{2\pi km}{n}\right)$$

We also have the inverse relation

$$\psi_m = \frac{1}{n} \sum_{k=0}^{n-1} |\hat{x}_k|^2 \exp\left(+i\frac{2\pi km}{n}\right)$$

To prove the latter relation, we first substitute the inverse DFT for x_j and x_{j+m} in the definition of ψ_m:

$$\begin{aligned} \psi_m &= \sum_{j=0}^{n-1} x_j^* x_{j+m} \\ &= \sum_{j=0}^{n-1} \left[\frac{1}{n} \sum_{k=0}^{n-1} \hat{x}_k^* \exp\left(-i\frac{2\pi kj}{n}\right) \right] \left[\frac{1}{n} \sum_{k'=0}^{n-1} \hat{x}_{k'} \exp\left(i\frac{2\pi k'(j+m)}{n}\right) \right] \end{aligned}$$

We then change the order of the summations and simplify as follows:

$$\psi_m = \frac{1}{n^2}\sum_{k=0}^{n-1}\sum_{k'=0}^{n-1}\hat{x}_k^*\hat{x}_{k'}\exp\left(i\frac{2\pi mk'}{n}\right)\underbrace{\sum_{j=0}^{n-1}\exp\left(i\frac{2\pi j(k'-k)}{n}\right)}_{\substack{=n,\;\; k'=k\\ =0,\;\; k'\neq k}}$$

$$= \frac{1}{n}\sum_{k=0}^{n-1}\hat{x}_k^*\hat{x}_k\exp\left(i\frac{2\pi mk}{n}\right)$$

which is the Wiener-Khintchin relation.

By Fourier transforming ψ_m we also prove the inverse relation: the power spectrum is the Fourier transform of the autocorrelation.

For a real time series $\{x_j\}$, we can use the previously derived relation

$$\hat{x}_k^* = \hat{x}_{n-k} = \hat{x}_{-k}$$

to show that

$$|\hat{x}_k|^2 = \hat{x}_k\hat{x}_k^* = \hat{x}_k\hat{x}_{n-k} = \hat{x}_{n-k}^*\hat{x}_{n-k} = |\hat{x}_{n-k}|^2.$$

This redundancy results from the fact that neither the autocorrelation nor the power spectrum contain information on any "phase lags" in either x_j or its individual frequency components.

Thus while the DFT of an n-point time series results in n independent quantities ($2\times n/2$ complex numbers), the power spectrum yields only $n/2$ independent quantities.

One may therefore show that there are an infinite number of time series that have the same power spectrum, but that each time series uniquely defines its Fourier transform, and vice-versa.

Consequently a time series cannot be reconstructed from its power spectrum or autocorrelation function.

1.4 Power spectrum of a periodic signal

Consider a periodic signal

$$x(t) = x(t+T) = x\left(t + \frac{2\pi}{\omega}\right)$$

Consider the extreme case where the period T is equal to the duration of the signal:

$$T = t_{\text{max}} = n\Delta t$$

The Fourier components are separated by

$$\Delta f = \frac{1}{t_{\text{max}}}$$

i.e. at frequencies

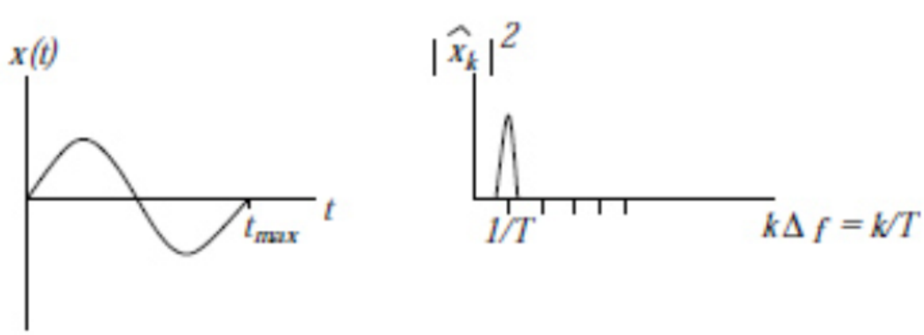
$$0,\ 1/T,\ 2/T, \ldots, (n-1)/T.$$

1.4.1 Sinusoidal signal

In the simplest case, $x(t)$ is a sine or cosine, i.e.,

$$x(t) = \sin\left(\frac{2\pi t}{t_{\text{max}}}\right).$$

What is the Fourier tranform? Pictorially, we expect



We calculate the power spectrum analytically, beginning with the DFT:

$$
\begin{aligned}
\hat{x}_k &= \sum_j x_j \exp\left(\frac{-i2\pi jk}{n}\right) \\
&= \sum_j \sin\left(\frac{2\pi j\Delta t}{t_{\max}}\right) \exp\left(\frac{-i2\pi jk}{n}\right) \\
&= \frac{1}{2i}\sum_j \left[\exp\left(\frac{i2\pi j\Delta t}{t_{\max}}\right) - \exp\left(\frac{-i2\pi j\Delta t}{t_{\max}}\right)\right] \exp\left(\frac{-i2\pi jk}{n}\right) \\
&= \frac{1}{2i}\sum_j \left[\exp\left\{i2\pi j\left(\frac{\Delta t}{t_{\max}} - \frac{k}{n}\right)\right\} - \exp\left\{-i2\pi j\left(\frac{\Delta t}{t_{\max}} + \frac{k}{n}\right)\right\}\right] \\
&= \pm\frac{n}{2i} \qquad \text{when } k = \frac{\pm n\Delta t}{t_{\max}}.
\end{aligned}
$$

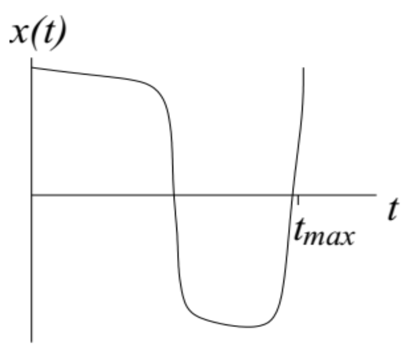
Thus

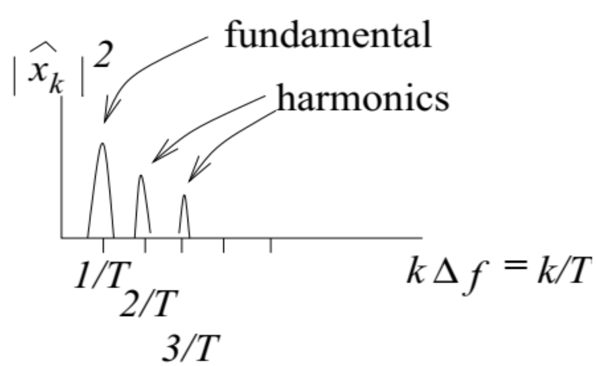
$$
|\hat{x}_k|^2 = \frac{n^2}{4} \qquad \text{for } k = \pm 1.
$$

1.4.2 Non-sinusoidal signal

Consider now a non-sinusoidal yet periodic signal, similar to that of the signals seen in glacial cycles.

The non-sinusoidal character of such oscillations implies that it contains higher-order *harmonics*, i.e., integer multiples of the *fundamental frequency* $1/T$. Thus, pictorially, we expect





Now suppose $t_{\max} = pT$, where p is an integer. The non-zero components of the power spectrum must still be at frequencies

$$1/T,\ 2/T, \ldots.$$

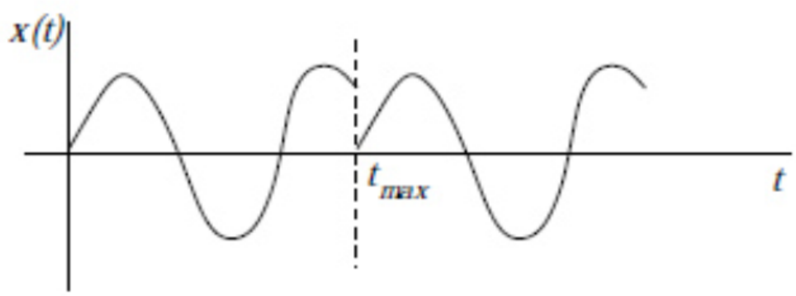
But since

$$\Delta f = \frac{1}{t_{\max}} = \frac{1}{pT}$$

the frequency resolution is p times greater. Contributions to the power spectrum would remain at integer multiples of the frequency $1/T$, but spaced p samples apart on the frequency axis.

1.4.3 $t_{\max}/T \neq$ integer

If $t_{\max}/T$ is not an integer, the (effectively periodic) signal looks like



We calculate the power spectrum of such a signal, assuming the sinusoidal function

$$x(t) = \exp\left(i\frac{2\pi t}{T}\right)$$

which has the discrete form

$$x_j = \exp\left(i\frac{2\pi j\Delta t}{T}\right).$$

The DFT is

$$\hat{x}_k = \sum_{j=0}^{n-1} \exp\left(i\frac{2\pi j\Delta t}{T}\right) \exp\left(-i\frac{2\pi jk}{n}\right).$$

Set

$$\phi_k = \frac{\Delta t}{T} - \frac{k}{n}.$$

Then

$$\hat{x}_k = \sum_{j=0}^{n-1} \exp\left(i2\pi\phi_k j\right).$$

Recall the identity

$$\sum_{j=0}^{n-1} x^j = \frac{x^n - 1}{x - 1}.$$

Then

$$\hat{x}_k = \frac{\exp(i2\pi\phi_k n) - 1}{\exp(i2\pi\phi_k) - 1}.$$

The power spectrum is

$$\begin{aligned} |\hat{x}_k|^2 = \hat{x}_k\hat{x}_k^* &= \frac{1 - \cos(2\pi\phi_k n)}{1 - \cos(2\pi\phi_k)} \\ &= \frac{\sin^2(\pi\phi_k n)}{\sin^2(\pi\phi_k)}. \end{aligned}$$

Note that

$$n\phi_k = \frac{n\Delta t}{T} - k = \frac{t_{\max}}{T} - k$$

is the difference between a DFT index k and the "real" non-integral frequency index $t_{\max}/T$.

Assume that n is large and k is close to that "real" frequency index such that

$$n\phi_k = \frac{n\Delta t}{T} - k \ll n.$$

Consequently $\phi_k \ll 1$, so we may also assume

$$\pi\phi_k \ll 1.$$

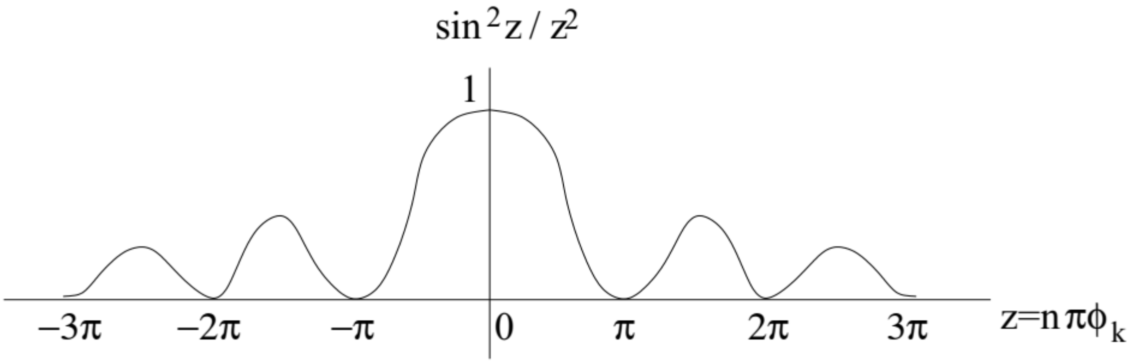
Then

$$\begin{aligned} |\hat{x}_k|^2 &\simeq \frac{\sin^2(\pi\phi_k n)}{(\pi\phi_k)^2} \\ &= n^2 \frac{\sin^2(\pi\phi_k n)}{(\pi\phi_k n)^2} \\ &\propto \frac{\sin^2 z}{z^2} \end{aligned}$$

where

$$z = n\pi\phi_k = \pi\left(\frac{n\Delta t}{T} - k\right) = \pi\left(\frac{t_{\max}}{T} - k\right).$$

Thus $|\hat{x}_k|^2$ is no longer a simple spike. Instead, as a function of $z = n\pi\phi_k$ it appears as



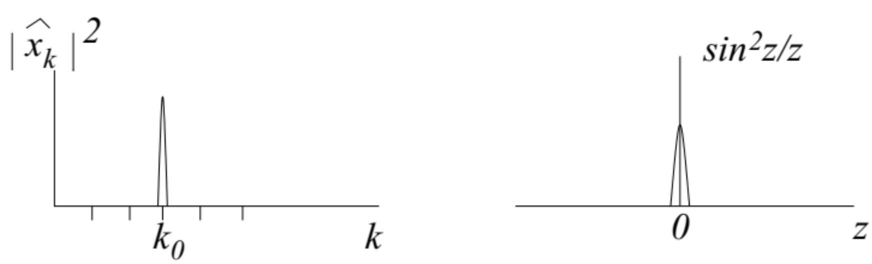
The plot gives the kth component of the power spectrum of $e^{i2\pi t/T}$ as a function of $\pi(t_{\max}/T - k)$.

To interpret the plot, let k_0 be the integer closest to $t_{\max}/T$. There are then two extreme cases:

1. $t_{\max}$ is an integral multiple of T:

$$\frac{t_{\max}}{T} - k_0 = 0.$$

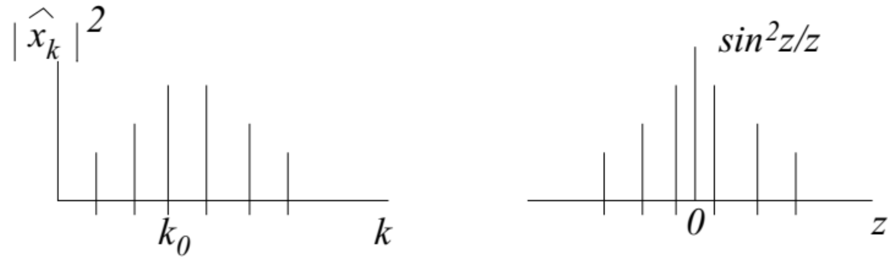
   The spectrum is perfectly sharp:



2. $t_{\max}/T$ falls midway between two frequencies. Then

$$\frac{t_{\max}}{T} - k_0 = \frac{1}{2}.$$

   The spectrum is smeared:



The smear decays like

$$\frac{1}{(k - t_{\max}/T)^2} \sim \frac{1}{k^2}$$

1.4.4 Conclusion

The power spectrum of a periodic signal of period T is composed of:

1. a peak at the frequency $1/T$
2. a smear (sidelobes) near $1/T$
3. possibly harmonics (integer multiples) of $1/T$
4. smears near the harmonics.