

PHYS 5319-001: Math Methods in Physics III

Discrete Fourier Transformation

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Fourier Analysis

- A single-valued period function (w/ period T)

$$y(t + T) = y(t)$$

can be expanded as

$$y(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos(n\omega t) + b_n \sin(n\omega t))$$

where “true” frequency $\omega = \frac{2\pi}{T}$

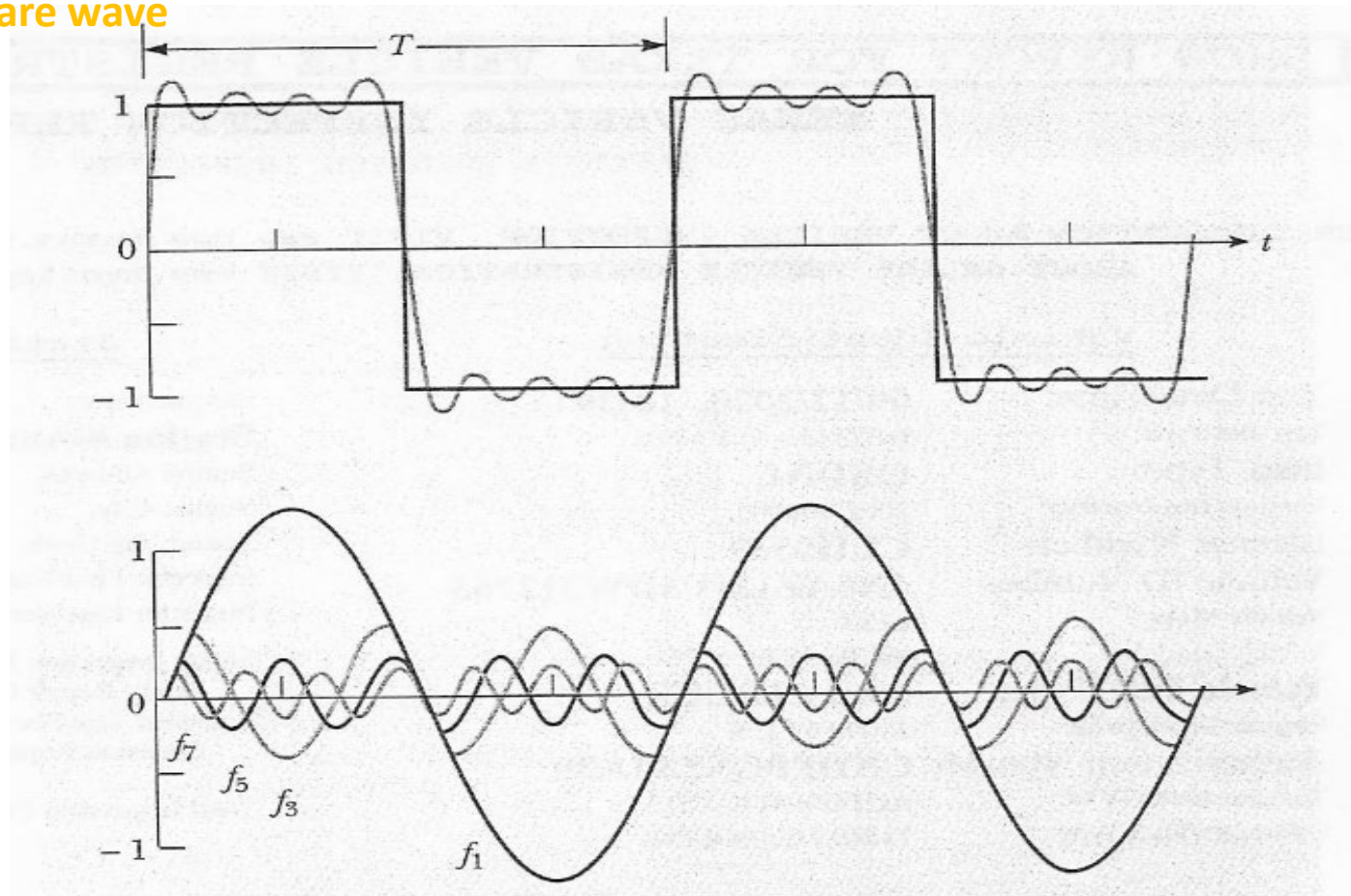
-given a $y(t)$ to find $\{a_n, b_n\}$: $\begin{pmatrix} a_n \\ b_n \end{pmatrix} = \frac{2}{T} \int_0^T dt \begin{pmatrix} \cos(n\omega t) \\ \sin(n\omega t) \end{pmatrix} y(t)$

* $a_0 = 2\langle y(t) \rangle$

*for odd , all $\{a_n\}=0$, $b_n = \frac{4}{T} \int_0^{T/2} dt y(t) \sin(n\omega t)$

* for even , all $\{b_n\}=0$, $a_n = \frac{4}{T} \int_0^{T/2} dt y(t) \cos(n\omega t)$

Example: Square wave



Odd function

$$a_0 = \{a_n\} = 0$$

$$b_n = \begin{cases} 0, & n = 2, 4, 6, 8, \dots \\ \frac{4}{n\pi}, & n = 1, 3, 5, 7, \dots \end{cases}$$

Here we truncated at $n=7$. The converge is slow.

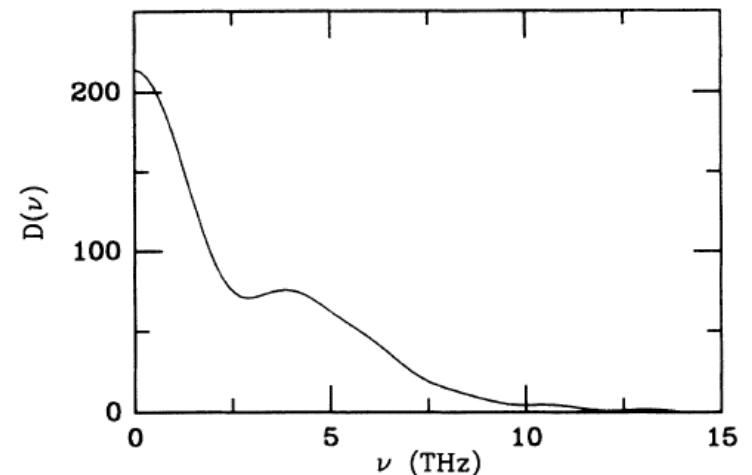
Autocorrelation function

- **Autocorrelation** is the correlation of a signal with a delayed copy of itself as a function of delay. Informally, it is the similarity between observations as a function of the time lag between them. The analysis of autocorrelation is a mathematical tool for finding repeating patterns, such as the presence of a periodic signal obscured by noise, or identifying the missing fundamental frequency in a signal implied by its harmonic frequencies.

e.g. Liquid GaAs, *Phys. Rev. B* 42, 5071 (1990)

$$Z(s) = \frac{\langle \mathbf{V}(t) \cdot \mathbf{V}(t + s) \rangle}{\langle \mathbf{V}(t) \cdot \mathbf{V}(t) \rangle}.$$

$$D(\nu) \propto \int_0^\infty Z(t) \cos(2\pi\nu t) dt,$$



In general, the fundamental freq. $\omega_1 = \frac{2\pi}{T}$

Then we have discrete frequency: $\omega_1, 2\omega_1, 3\omega_1, \dots$

$$\text{with } \Delta\omega = \omega_1 = \frac{2\pi}{T}$$

For a nonperiodic function, we can imagine $T \rightarrow \infty$

Then $\Delta\omega \rightarrow 0$ or ω becomes continuous:

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

For comparison:

$$y(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos(n\omega t) + b_n \sin(n\omega t))$$

$$e^{i\omega t} = \cos\omega t + i\sin\omega t$$

Here $Y(\omega)$ replace $\{a_n, b_n\}$, called Fourier Transform of $y(t)$

A plot $|Y(\omega)|^2$ of vs. ω is usually called the power spectrum

Inverse F.T.:
$$y(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega Y(\omega) e^{i\omega t}$$

forward F.T.:
$$Y(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt y(t) e^{-i\omega t}$$

Know either of them can get another. Sometimes experiments may well measure $Y(\omega)$ directly.

Also, note
$$\frac{d}{dt} y(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \underline{Y(\omega)(i\omega)} e^{i\omega t}$$

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

Discrete Fourier Transform

For a periodic function

finite $y_k \equiv y(t_k), k = 0, 1, 2, \dots, N$



Since $y(t+T)=y(t) \Rightarrow y_0 = y_N$

$$T = Nh$$

Prime freq.: $\omega_1 = \frac{2\pi}{T}$

$$\omega_n = n\omega_1 = n \frac{2\pi}{Nh}, n = 0, 1, \dots, N$$

$$t_k = kh$$

Higher frequency contribution is missing \Rightarrow more rapid change

$$FT \quad Y(\omega_n) = \frac{1}{T} \int_0^T e^{-i\omega_n t} y(t) dt \approx \frac{1}{T} \sum_{k=1}^N y(t_k) e^{-i\omega_n t_k h} = \frac{1}{N} \sum_{k=1}^N y_k e^{-i2\pi kn/N}$$

usually:

$$Y_n \equiv \sum_{k=1}^N y_k e^{-2\pi i kn/N}$$

$$FT^{-1} \quad y_k \equiv \frac{1}{N} \sum_{n=1}^N Y_n e^{2\pi i kn/N}$$

multi-grid
fine - coarse

DFT recap

$$Y_n \equiv \sum_{k=1}^N y_k e^{-2\pi i k n / N}$$

$$y_k \equiv \frac{1}{N} \sum_{n=1}^N Y_n e^{2\pi i k n / N}$$

Periodic:

$$Y_{\underline{n+N}} = Y_n$$

$$y_{k+N} = y_k$$

N independent input \Rightarrow N independent output

Let $Z \equiv e^{2\pi i / N}$

$$e^{2\pi i k n / N} = Z^{kn}$$

Z could be pre-calculated

Cost of DFT: for each $Y_n \equiv \sum_{k=1}^N y_k * Z^{kn}$, about $O(N)$

But $n=1,2,\dots,N$. So we have N Y_n 's to calculate, the total operation $\sim O(N^2)$

An algorithm called Fast Fourier Transformation (FFT) will reduce it to $O(N \log_2 N)$

Similarly, in 1-d real space, we have a periodic function $f(x + L) = f(x)$

Discrete Fourier Transform (DFT)

$$f_i, i = 1, 2, \dots, N$$

FT

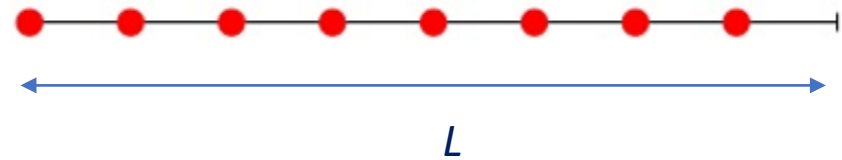
$$\begin{aligned} g(k) &= \frac{1}{L} \int_0^L f(x) e^{ikx} dx \\ &= \frac{1}{N} \sum_{j=1}^N f_j e^{ikx_i} \end{aligned}$$

FT⁻¹

$$f(x) = \sum_{l=1}^N g_l e^{-ik_l x}$$

N discrete points:

$$x = 0, \frac{L}{N}, \frac{2L}{N}, \dots, \frac{L}{N}(N-1)$$



Since $f(x+L)=f(x) \Rightarrow e^{ikL}=1$,
 $kL = 2\pi n, n = 0, 1, 2, \dots, N-1$

We have N discrete k-points:

$$k = \frac{2\pi n}{L}, n = 0, 1, 2, \dots, N-1$$

Fast Fourier Transformation

- Idea by Gauss (1886); developed by Cooley & Tukey (1965)
- "the most important numerical algorithm of our lifetime"

For $N=2^m$,

$$\begin{aligned} y_n &= \sum_{k=0}^{N-1} Y_k e^{2\pi i k n / N} \\ &= \sum_{k=0}^{\frac{N}{2}-1} Y_{2k} e^{i2\pi 2kn/N} + \sum_{k=0}^{\frac{N}{2}-1} Y_{2k+1} e^{i2\pi(2k+1)n/N} \end{aligned}$$

Split the FT into odd/even terms

$$\begin{aligned}y_n &= \sum_{k=0}^{N-1} Y_k e^{2\pi i k n / N} \\&= \sum_{k=0}^{\frac{N}{2}-1} Y_{2k} e^{i2\pi 2kn/N} + \sum_{k=0}^{\frac{N}{2}-1} Y_{2k+1} e^{i2\pi(2k+1)n/N} \\&= x_n + z_n e^{i2\pi n/N}\end{aligned}$$

where $x_n = \sum_{k=0}^{\frac{N}{2}-1} Y_{2k} e^{i2\pi kn / (\frac{N}{2})}$, $z_n = \sum_{k=0}^{\frac{N}{2}-1} Y_{2k+1} e^{i2\pi kn / (\frac{N}{2})}$

Let $w = e^{i2\pi/N}$, then $y_n = x_n + w^n z_n$

x_n and z_n has period of $N/2$

This is very significant!

$$y_n = x_n + w^n z_n$$

x_n and z_n has period of $N/2$

$$\text{i.e. } x_0 = x_{N/2}, z_0 = z_{N/2}$$

Can be done recursively: $N \rightarrow \frac{N}{2} \rightarrow \frac{N}{4} \rightarrow \dots \rightarrow 2$

Total cost $O(N \log_2 N)$