Computational Physics – Lecture 19

(27 April 2020)

Recap

In the previous class, we learnt how to convolve and deconvolve two functions numerically.

Today's plan

In today's class, we want to learn something called spectral analysis of functions.

Introduction

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Power spectral estimation also has theoretical applications in study of stochastic quantities, e.g., in statistical mechanics, astrophysics, and cosmology.

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Every physical phenomenon – electromagnetic, thermal, mechanical, etc. – has an associated spectrum.

In Fourier analysis, we split a function into frequency components. So Fourier transforms give a natural way to generalise the notion of a spectrum to arbitrary functions.

Parseval's theorem

Parseval's theorem says that

$$\int_{-\infty}^{\infty} \mathrm{d}x\ f_1(x)[f_2(x)]^* = \int_{-\infty}^{\infty} \mathrm{d}k\ \tilde{f}_1(k)[\tilde{f}_2(k)]^*. \tag{1}$$

This is because

$$\begin{aligned}
&\int_{-\infty}^{\infty} \mathrm{d}x\ f_1(x)[f_2(x)]* & (2)\\
&= \int_{-\infty}^{\infty} \mathrm{d}x\ \left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}k \cdot \tilde{f}(k) \cdot \exp(ikx)\right][f_2(x)]^* & (3)\\
&= \int_{-\infty}^{\infty} \mathrm{d}x\ \left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}k \cdot \tilde{f}_1(k) \cdot \exp(ikx)\right][f_2(x)]^* & (4)\\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}k \cdot \tilde{f}_1(k)\left[\int_{-\infty}^{\infty} \mathrm{d}x \exp(ikx)[f_2(x)]^*\right] & (5)\\
&= \int_{-\infty}^{\infty} \mathrm{d}k \cdot \tilde{f}_1(k)[\tilde{f}_2(k)]^* & (6)\\
& & (7)
\end{aligned}$$

Power spectrum

So now if $f_1 = f_2$, we have

$$\int_{-\infty}^{\infty} \mathrm{d}x \; |f_1(x)|^2 = \int_{-\infty}^{\infty} \mathrm{d}k \; |\tilde{f}_1(k)|^2. \tag{8}$$

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The function $|\tilde{f}_1(k)|^2$, which is a function of k, is called the *power spectrum* or the *power spectral density* of $f(x)$.

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The function $|\tilde{f}_1(k)|^2$, which is a function of k, is called the *power spectrum* or the *power spectral density* of $f(x)$.

The *average power* over a scale X is defined as

$$p_{\mathrm{avg}} = \frac{1}{X} \int_0^X \mathrm{d}x \, |f^2(x)|. \tag{9}$$

Random functions

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Or, $f(x)$ could describe a fundamentally stochastic quantity such as a quantum field or the cosmological matter distribution.

In such cases $f(x)$ is a random variable with a certain probability distribution.

Random functions

But then the quantity

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x \cdot f(x) \cdot \exp(-ikx)$$

is also a random variable.

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"If the signal has non-zero power, it has infinite energy. If it has finite energy, it has zero average power."

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In such cases, we study *statistics in Fourier space*.

Power spectrum of a random function

We can begin by defining a truncated function

$$f_X(x) = \begin{cases} f(x) & \text{if } |x| \leq X \\ 0, & \text{otherwise,} \end{cases} \tag{10}$$

so that

$$f(x) = \lim_{X \to \infty} f_X(x).$$

No $f_X(x)$ satisfies the Dirichlet condition and a Fourier transform exists.

Power spectrum of a random function

Now we know from Parseval's theorem that

$$\int_{-\infty}^{\infty} \mathrm{d}x \; |f_X(x)|^2 = \int_{-\infty}^{\infty} \mathrm{d}k \; |\tilde{f}_X(k)|^2. \tag{11}$$

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We still cannot take the limit $X \to \infty$ because the Fourier transform does not exist in that limit.

Power spectrum of a random function

But we can take the expectation value.

$$E\left\{\frac{1}{2X}\int_{-\infty}^{\infty}\mathrm{d}x\,|f_X(x)|^2\right\} = E\left\{\frac{1}{2X}\int_{-\infty}^{\infty}\mathrm{d}k\,|\tilde{f}_X(k)|^2\right\}. \quad (13)$$

which gives us

$$\frac{1}{2X}\int_{-\infty}^{\infty}\mathrm{d}x\,E\left\{|f_X(x)|^2\right\} = \frac{1}{2X}\int_{-\infty}^{\infty}\mathrm{d}k\,E\left\{|\tilde{f}_X(k)|\right\}^2. \quad (14)$$

or

$$\lim_{X\to\infty}\frac{1}{2X}\int_{-\infty}^{\infty}\mathrm{d}x\,\bar{f}^2(x) = \lim_{X\to\infty}\frac{1}{2X}\int_{-\infty}^{\infty}\mathrm{d}k\,E\left\{|\tilde{f}_X(k)|\right\}^2. \quad (15)$$

which gives

$$\langle\bar{f}^2(x)\rangle = \int_{-\infty}^{\infty}\mathrm{d}k\,\lim_{X\to\infty}\frac{E\left\{|\tilde{f}_X(k)|\right\}^2}{2X}. \quad (16)$$

(Bar: ensemble average; Angle brackets: time average)

Power spectrum of a random function

Time average of the ensemble rms value is just the rms value so

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$$P(k) = \lim_{X \to \infty} \frac{E\left\{|\tilde{f}_X(k)|\right\}^2}{2X}$$

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Remember that

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We have discovered a simple connection between the power spectrum and statistics.

Wiener-Khinchin Theorem

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We have

$$P(k) = \lim_{X\to\infty} \frac{E\left\{|\tilde{f}_X(k)|\right\}^2}{2X} \tag{18}$$

$$= \lim_{X\to\infty} \frac{1}{2X} E\left\{\left[\int_{-\infty}^{\infty} dx_1 f_X(x_1) \exp\left(-ikx_1\right)\right]\right. \tag{19}$$

$$\left.\left[\int_{-\infty}^{\infty} dx_2 f_X(x_2) \exp\left(ikx_2\right)\right]\right\} \tag{20}$$

where we have used the fact that

$$|\tilde{f}_X(k)|^2 = f_X(k) f_X(-k)$$

Wiener-Khinchin Theorem

The above will give us

$$P(k) = \lim_{X\to\infty} \frac{1}{2X} \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dx_1 \left\{ E\left[f_X(x_1) f_X(x_2) \right] \right. \\ \left. \times \exp\left(ik(x_2 - x_1) \right) \right\} \tag{21}$$

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The quantity $E\left[f_X(x_1) f_X(x_2)\right]$ is called the *correlation function.*

$$E\left[f_X(x_1) f_X(x_2)\right] = \begin{cases} R(x_1, x_2), & \text{if} |x_1|, |x_2| < X \\ 0, & \text{otherwise}, \end{cases} \tag{22}$$

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Wiener-Khinchin Theorem

If we write $x_2 - x_1 = \xi$ and $dx_2 = d\xi$, we get

$$P(k) = \int_{-\infty}^{\infty} d\xi \left[\lim_{X \to \infty} \frac{1}{2X} \int_{-X}^{X} dx_1 R(x_1, x_1 + \xi) \right. \\ \left. \times \exp\left(-ik\xi\right) \right] . \tag{23}$$

So the power spectrum is the Fourier transform of the time-averaged correlation function!

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Wiener-Khinchin Theorem

For isotropic or stationary processes, the correlation function is independent of x so

$$\langle R(x_1, x_1 + \xi) \rangle = R(\xi), \tag{24}$$

and we get

$$\tilde{P}(k) = \int_{-\infty}^{\infty} \mathrm{d}x \cdot R(x) \cdot \exp(-ikx) \tag{25}$$

and

$$R(x) = \int_{-\infty}^{\infty} \mathrm{d}k \cdot \tilde{P}(k) \cdot \exp(ikx). \tag{26}$$

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But if $f(x)$ is a random function, we now know that the power spectrum measures statistics of the distribution from which $f(x)$ is derived.

Computation

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But if $f(x)$ is a random function, we now know that the power spectrum measures statistics of the distribution from which $f(x)$ is derived.

How well does the DFT-based computation approximate those statistics?

Estimators

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For example

$$\hat{m} = \frac{1}{n} \sum_{0}^{n-1} x_n \tag{27}$$

is an estimator for the mean.

Good and bad estimators

An estimator is good, or consistent, if

- its expectation value is equal to the true value of the statistic that it is measuring
- its variance is small

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For example, the above estimator for the mean is consistent. But the estimator

$$S^2 = \frac{1}{n} \sum (x_i - \bar{x})^2 \tag{28}$$

is not a consistent estimator for variance. (It is biased.) The estimator

$$S^2 = \frac{1}{n-1} \sum (x_i - \bar{x})^2 \tag{29}$$

is consistent.

Periodogram

We can start by defining a power spectrum estimator as

$$P_n(k_q) = \frac{1}{n} |\tilde{f}(k_q)|^2 \tag{30}$$

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Suppose we also discretise the correlation function as

$$R_n(p) = \frac{1}{n}\sum f_r \cdot f_{r+p} \tag{31}$$

Periodogram

Then we have

$$
\begin{aligned}
P_n(q) &= \sum R_n(p) \cdot \exp\left(\frac{-i2\pi qp}{n}\right) \\
&= \sum \left[\frac{1}{n}\sum f_r \cdot f_{r+p}\right] \cdot \exp\left(\frac{-i2\pi qp}{n}\right) \\
&= \frac{1}{n}\left[\sum f_n \exp\left(\frac{i2\pi qr}{n}\right)\right] \cdot \left[\sum f_{r+p} \exp\left(\frac{-i2\pi q(r+p)}{n}\right)\right] \\
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What is the expectation value of $R_n(p)$?

It is given by

$$E\left[R_n(p)\right] = \left(1 - \frac{|p|}{n}\right) R(p), \tag{34}$$

where $R(p)$ is the true correlation function $E\left[f(x_r) f(x_r + p\Delta)\right]$

Periodogram

Let us denote

$$a(p) = \left(1 - \frac{|p|}{n}\right) \tag{35}$$

then we have

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Using the discrete convolution theorem, this means that

$$E\left[P_n(q)\right] = \sum P(s)A(q-s) \tag{37}$$

where A is the Fourier transform of a and is of the form

$$A(k) \propto \left[\frac{\sin 2\pi kn/2}{\sin 2\pi k/2}\right]^2 \tag{38}$$

So the estimator is biased but becomes asymptotically unbiased for $n \to \infty$.

Periodogram

But the variance of $P_n(q)$ can be shown to give $P^2(q)$

$$\lim_{n\to\infty} \mathrm{var}\left[P_n(q)\right] = P^2(q), \tag{39}$$

so our estimator, the periodogram, is not consistent.

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Many solutions to this problem have been proposed.

One such solution is the Bartlett method.

Note that $x_1, x_2, \ldots, x_l$ are uncorrelated random variables with mean $E(X)$ and variance σ^2 then the quantity

$$\frac{x_1 + x_2 + \ldots + x_l}{l} \tag{40}$$

has mean $E(X)$ and variance σ^2/l.

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For the averaged periodogram the bias will go to zero and the variance will go to zero as $l \to \infty$.

This is therefore a consistent method of deriving the power spectrum.

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Higher-dimensional FTs are straitforward to define. For example

$$\tilde{f}(k) = \frac{1}{(\sqrt{2\pi})^2} \int_{-\infty}^{\infty} \mathrm{d}x_1 \int_{-\infty}^{\infty} \mathrm{d}x_2 \cdot f(x_1, x_2) \cdot \exp(-i(k_1 x_1 + k_2 x_2))$$

and its discrete version

$$\tilde{f}_{qr} = \frac{1}{\sqrt{mn}} \sum \sum f_{ps} \exp\left(-i2\pi \left[\frac{pq}{n} + \frac{rs}{m}\right]\right).$$

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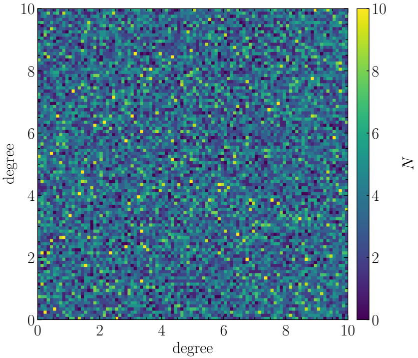
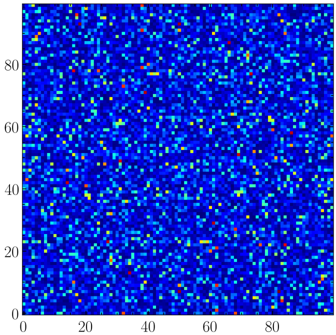
Coding higher-dimensional DFT is hard! But libraries are available.

2d power spectrum



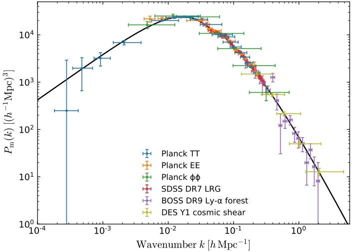
A poisson-distributed field.

2d power spectrum



2d power spectrum of the previous field.

3d power spectrum



3d power spectrum of the matter distribution in the universe.

What we have learnt so far

- Fourier transform, Fourier series, and Discrete Fourier transform
- Fast Fourier Transform algorithm
- DFT as a means to compute the FT
- Convolution and deconvolution of functions
- Optimal filtering
- Power spectra and statistics
- Higher-dimensional FTs