Fourier Analysis

- One of the most useful tools in theoretical and computational physics.
- Wide range of physics and math applications:
  - Spectral analysis
  - Signal processing
  - Solving differential equations (ODE and PDE)
  - Interpolation, and more.
- Widely used in modern technology (e.g. sound, image and video compression).

Fourier Analysis: Motivation

- Taylor series expansion of a function is a very useful and powerful tool, as we have seen throughout this course (and many others).
- However, it has certain important limitations:
  - Not suitable for periodic functions (unique point).
  - Cannot handle discontinuities (all derivatives should exist).
- Both issues addressed by the Fourier series representation of a function.

Fourier series

- The origin of the Fourier analysis lies in Fourier series expansion.
- Any periodic function with a finite number of discontinuities on a finite interval 0<x<L can be represented in Fourier series:

$$f(x) = \sum_{k=0}^{\infty} \alpha_k \cos\left(\frac{2\pi kx}{L}\right) + \sum_{k=1}^{\infty} \beta_k \sin\left(\frac{2\pi kx}{L}\right) = \sum_{k=-\infty}^{\infty} \gamma_k \exp\left(i\frac{2\pi kx}{L}\right)$$

where we set:

$$\gamma_k = \begin{cases} \frac{1}{2}(\alpha_{-k} + i\beta_{-k}), & k < 0 \\ \alpha_0, & k = 0 \\ \frac{1}{2}(\alpha_k - i\beta_k), & k > 0 \end{cases}$$

and used that:

$$e^{i\theta} = \cos\theta + i\sin\theta \Longleftrightarrow \cos\theta = \frac{1}{2}(e^{-i\theta} + e^{i\theta}), \sin\theta = \frac{i}{2}(e^{-i\theta} - e^{i\theta})$$

Fourier series

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Dirichlet's theorem: *If $f(t)$ is periodic of period 2π, if for $-\pi < t < \pi$ the function $f(t)$ has a finite number of maximum and minimum values and a finite number of discontinuities, and if $\int_{-\pi}^{\pi} f(t)\,dt$ is finite, then the Fourier series converges to $f(t)$ at all points where $f(t)$ is continuous, and at jump-points it converges to the arithmetic mean of the right-hand and left-hand limits of the function.*

$$f(x) = \sum_{k=0}^{\infty} \alpha_k \cos\left(\frac{2\pi k x}{L}\right) + \sum_{k=1}^{\infty} \beta_k \sin\left(\frac{2\pi k x}{L}\right) = \sum_{k=-\infty}^{\infty} \gamma_k \exp\left(i\frac{2\pi k x}{L}\right)$$

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and used that:

$$e^{i\theta} = \cos\theta + i\sin\theta \iff \cos\theta = \frac{1}{2}(e^{-i\theta} + e^{i\theta}), \sin\theta = \frac{i}{2}(e^{-i\theta} - e^{i\theta})$$

Fourier series (cont.)

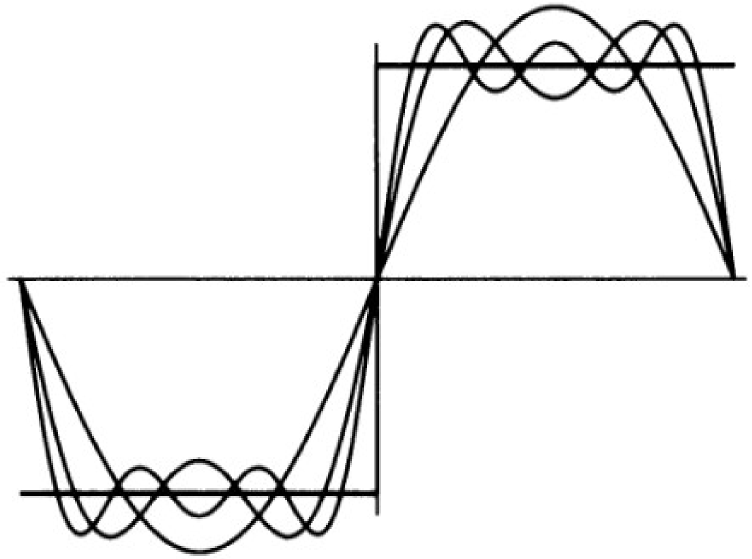
- How do we calculate γ_k? (Check the math!)

$$\gamma_k = \frac{1}{L}\int_0^L f(x)\exp\left(-i\frac{2\pi k x}{L}\right)dx$$

- Notes:
  - Fourier series can also represent discontinuous functions (unlike e.g. Taylor series)
  - What about non-periodic functions? → Make them periodic!

  → Some examples next.

Example: step function



$$f(t) = \begin{cases} -1, & t < 0 \\ +1, & t > 0 \end{cases}$$

$$\begin{aligned} b_n &= \frac{1}{\pi}\int_{-\pi}^{0}(-1)\sin nt\,dt + \frac{1}{\pi}\int_{0}^{\pi}(+1)\sin nt\,dt \\ &= \frac{2}{\pi}\int_0^{\pi}\sin nt\,dt \\ &= \frac{2}{n\pi}[1-\cos n\pi] \\ &= \begin{cases} 0, & n = 2,4,6,\ldots \\ 4/n\pi, & n = 1,3,5,\ldots \end{cases}. \end{aligned}$$

This series of successive approximations provides the best possible fit to the original function,improving with every successive term.

How do we make a function periodic?

- We want to construct series for a function over $0<x<L$.
- Simply repeat it outside that interval → becomes periodic (remember jumps are OK!)
- Data outside $0<x<L$ is discarded (we do not try to expand it in series there, so it is not relevant).

Fourier transform

- The continuous version of the Fourier series is the Fourier transform:

$$\mathfrak{F}[f(t)] = g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt$$

Forward

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

Inverse

Properties of the Fourier transform

$$\mathfrak{F}[f_1 + f_2] = \mathfrak{F}[f_1] + \mathfrak{F}[f_2]$$

→ linear

$$\mathfrak{F}[f(\alpha t)] = \frac{1}{|\alpha|} g\left(\frac{\omega}{\alpha}\right)$$

$$\mathfrak{F}^{-1}[g(\beta\omega)] = \frac{1}{|\beta|} f\left(\frac{t}{\beta}\right)$$

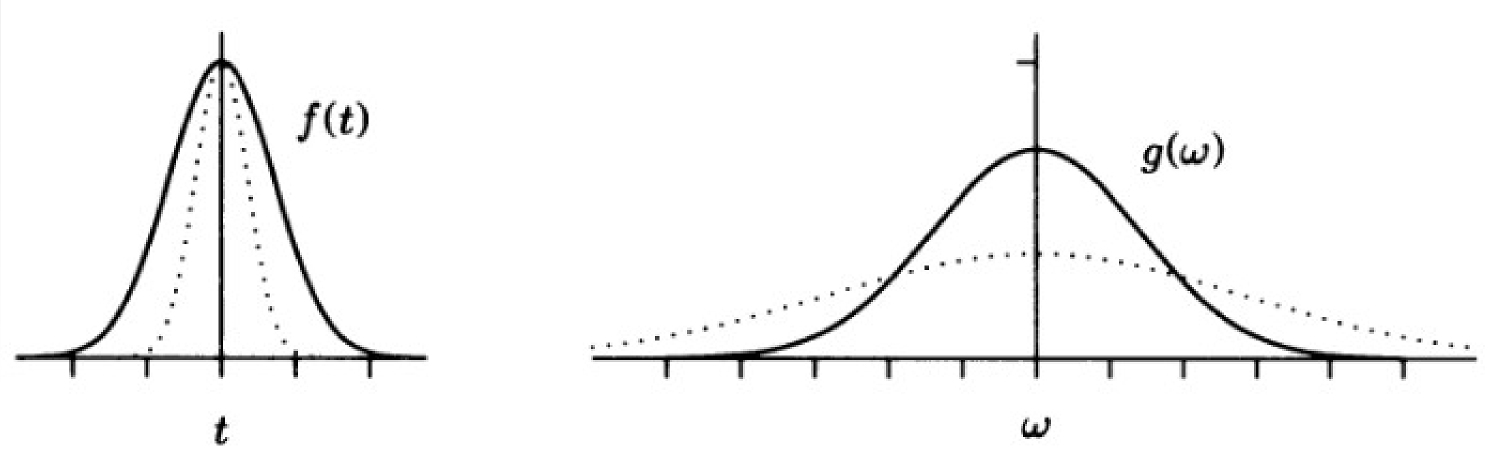
→ scaling relations

$$\mathfrak{F}[f(t - t_0)] = e^{-i\omega t_0} g(\omega)$$

$$\mathfrak{F}^{-1}[g(\omega - \omega_0)] = e^{i\omega_0 t} f(t)$$

→ phase shifts

Fourier transform: properties



- The broader f(t) is, the narrower g(ω) and vice-versa
- Related to the Heisenberg's Uncertainty Principle in Quantum Mechanics.

$$\Delta x \Delta p > h/2\pi$$

Discrete Fourier Transform

$$\gamma_k = \frac{1}{L}\int_0^L f(x)\exp\left(-i\frac{2\pi kx}{L}\right)dx$$

Q: How do we calculate γ_k in practice?

- For some f(x) one can do this exactly, but typically that is not possible.
- Use numerical integration, instead.

Discrete Fourier Transform (cont.)

- Applying e.g. the trapezoidal rule, we have:

$$\gamma_k = \frac{1}{L}\frac{L}{N}\left[\frac{1}{2}f(0) + \frac{1}{2}f(L) + \sum_{n=1}^{N-1} f(x_n)\exp\left(-i\frac{2\pi k x_n}{L}\right)\right]$$

where $x_n = nL/N$.

- Taking into account that f(0)=f(L) (periodic), we get:

$$\gamma_k = \frac{1}{N}\sum_{n=0}^{N-1} f(x_n)\exp\left(-i\frac{2\pi k x_n}{L}\right)$$

Discrete Fourier Transform (cont.)

- The typical situation is to have sampled signal $x_n \rightarrow y_n$ (e.g. in a lab experiment measuring something at regular time intervals), giving:

$$\gamma_k = \frac{1}{N} \boxed{\sum_{n=0}^{N-1} y_n \exp\left(-i\frac{2\pi k x_n}{L}\right)}$$

c_k : Fourier coefficients

- This is called Discrete Fourier Transform (DFT) of the samples y_n

Discrete Fourier Transform (DFT)

- Even though the trapezoidal rule we used to derive DFT is an approximation to the integrals, the DFT is in certain sense exact.
- To show this, recall the geometric series:

$$\sum_{k=0}^{N-1} a^k = \frac{1-a^N}{1-a},$$ and set $a = e^{i2\pi m/N}$

which gives (why?):

$$\sum_{k=0}^{N-1} e^{i2\pi km/N} = \frac{1-e^{i2\pi m}}{1-e^{i2\pi m/N}} = \begin{cases} 0, m \neq 0 \\ N, m = 0 \end{cases}$$

Discrete Fourier Transform (DFT)

- Coming back to DFT, consider the sum:

$$\sum_{k=0}^{N-1} c_k \exp\left(i\frac{2\pi kn}{N}\right) = \sum_{k=0}^{N-1}\sum_{m=0}^{N-1} y_m \exp\left(-i\frac{2\pi km}{N}\right)\exp\left(i\frac{2\pi kn}{N}\right)$$

$$= \sum_{m=0}^{N-1} y_m \sum_{k=0}^{N-1} \exp\left(i\frac{2\pi k(n-m)}{N}\right)$$

but the last sum is the same we just calculated above, (if we replace m→n-m), i.e. is equal to N, so:

$$y_n = \frac{1}{N}\sum_{k=0}^{N-1} c_k \exp\left(i\frac{2\pi kn}{N}\right)$$

Discrete Fourier Transform (DFT)

$$y_n = \frac{1}{N} \sum_{k=0}^{N-1} c_k \exp\left(i \frac{2\pi k n}{N} \right)$$

- This is the inverse DFT, which means that given the Fourier coefficients c_k we can recover the original data points y_n exactly (with arbitrary precision), i.e. c_k and y_n are equivalent datasets.

Discrete Fourier Transform (DFT)

- DFT is similar to the Fourier series, but not the same:
  - Sum is not infinite
  - Most importantly, function is given only at the sample points y_n and nowhere else – in-between the samples function could be doing anything and DFT will be the same.

Therefore, for proper representation we need good enough sampling and a reasonably smooth function.

Discrete Fourier Transform (DFT)

- This is also related to so-called aliasing, as follows:
  - The highest frequency that DFT can sample is $(N-1)\Delta\omega$, $\Delta\omega=2\pi/T$
  - In fact, the highest one is really $(N/2)\Delta\omega$ since the frequencies $(N/2)\Delta\omega$ to $(N-1)\Delta\omega$ are the same as $-(N/2)\Delta\omega$ to $-\Delta\omega$.
  - If f(t) is periodic in t, its Fourier transform is periodic in ω.
- This highest frequency that can be represented is called Nyquist frequency: $\omega_{Nyquist}=(N/2)\Delta\omega$

Discrete Fourier Transform (DFT)

- The aliasing and the Nyquist frequency have a simple physical meaning:

  e.g. if we have a periodic function with period T=1s and we sample it every 2s it will appear to be constant.

  Q: What happens if we sample it every 1.5s?

- Therefore, we need sufficiently frequent sampling for faithful representation.

DFT: properties

All results up to now apply equally whether f(x) is real or complex function. However, esp. in physics, f(x) is typically real, e.g. a signal we measure. This yields some simplifications:

Let y_n be real numbers and consider c_k for some N/2<k<N. Then, k=N-r, where 1≤r<N/2 and we have:

$$\begin{aligned} c_{N-r} &= \sum_{n=0}^{N-1} y_n \exp\left(-i\frac{2\pi(N-r)n}{N}\right) \\ &= \sum_{n=0}^{N-1} y_n \exp(-i2\pi n)\exp\left(i\frac{2\pi rn}{N}\right) \\ &= \sum_{n=0}^{N-1} y_n \exp\left(i\frac{2\pi rn}{N}\right) = c_r^* \end{aligned}$$

(using $e^{-i2\pi n}=1$ and y_n being real)

→ c_{N-r} and c_r are complex conjugates

→ we really need only calculate ck for 0≤ k≤N/2

If f(x) is complex we still need to calculate all c_k's.

Sample DFT Python code and usage

```
from numpy import zeros,loadtxt
from pylab import plot,xlim,show
from cmath import exp,pi

def dft(y):
    N = len(y)
    c = zeros(N//2+1,complex)
    for k in range(N//2+1):
        for n in range(N):
            c[k] += y[n]*exp(-2j*pi*k*n/N)
    return c
y = loadtxt("pitch.txt",float)
c = dft(y)
plot(abs(c))
xlim(0,500)
show()
```

← cmath – same as math, but can handle complex numbers

← DFT code

usage: read in a text file containing a signal to be analysed

← calculate and plot the Fourier coefficients

Note: this code is simple, but computationally expensive and thus slow (why?)

Fourier transforms in 2D and 3D

- How do we do higher-dimensional (2D, 3D) Fourier transforms?
- Useful in e.g. image processing, solving equations in 2D, 3D domains.

  → just do transforms in each direction in turn.

- Let's consider MxN grid of samples y_{mn}. We first transform each of the M rows:

$$c'_{ml} = \sum_{n=0}^{N-1} y_{mn} \exp\left(-i\frac{2\pi l n}{N}\right)$$

  → N coefficients for each row m, one for each l.

Fourier transforms in 2D and 3D

- Next, we take ℓ^{th} coefficient in each of the M rows and transform these:

$$c_{kl} = \sum_{m=0}^{M-1} c'_{mn} \exp\left(-i\frac{2\pi km}{N}\right)$$

- The two steps could be combined to give:

$$c_{kl} = \sum_{m=0}^{M-1}\sum_{n=0}^{N-1} y_{mn} \exp\left[-i2\pi\left(\frac{km}{M}+\frac{ln}{N}\right)\right]$$

with corresponding inverse transform:

$$y_{mn} = \frac{1}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1} c'_{kl} \exp\left[-i2\pi\left(\frac{km}{M}+\frac{ln}{N}\right)\right]$$

Physical meaning of the Fourier transform

- The Fourier transform breaks each function into a sum of simple sinusoidal waves (real or complex) – these could be spatial ones or temporal (or both) called modes.
- The magnitude (absolute value) of the coefficients of those waves give how important each particular frequency is → spectral analysis of the signal/image, etc.
- These typically include main frequency/frequencies, harmonics and noise.

Fast Fourier Transform (FFT)

- As seen, Fourier transforms are quite useful in a wide range of physical and technical applications.
- However, their calculation is quite computationally expensive and thus slow, even in the case of DFT (itself much cheaper than the full FT).

$$c_k = \sum_{n=0}^{N-1} y_n \exp\left(-i\frac{2\pi kn}{N}\right)$$

→ calculating each Fourier coefficient (single point in Fourier/frequency space!) takes N operations, or NxN=N^2 for all N points.

Fast Fourier Transform (FFT)

- In 2D or 3D this still more expensive – number of operations scales as N^4 and N^6, respectively.
- How large problems are practical to do? Depends on your computer, but as a rule of thumb let's say 10^9 operations are reasonable. So we can do about 30,000 points – i.e. not too many, about 1 second worth of music.
- In 2D/3D things are still much worse, we can do just 178/32 samples per dimension.

What can we do to improve this?

Fast Fourier Transform (FFT)

- Need a better algorithm! Fortunately it exists – FFT
- History note: first derived by Gauss in 1805, reinvented and improved several times since then.
- Method is simplest for $N=2^m$ points, so let's consider that:
  - Divide the points into odd and even (always possible)
  - The even terms give:

$$E_k = \sum_{r=0}^{\frac{1}{2}N-1} y_{2r} \exp\left(-i\frac{2\pi k(2r)}{N}\right) = \sum_{r=0}^{\frac{1}{2}N-1} y_{2r} \exp\left(-i\frac{2\pi kr}{N/2}\right)$$

$\rightarrow$ again a DFT, but with just N/2 points.

Fast Fourier Transform (FFT)

- FFT algorithm (cont.)

$$E_k = \sum_{r=0}^{\frac{1}{2}N-1} y_{2r} \exp\left(-i\frac{2\pi k(2r)}{N}\right) = \sum_{r=0}^{\frac{1}{2}N-1} y_{2r} \exp\left(-i\frac{2\pi kr}{N/2}\right)$$ → even

  - The odd terms give:

$$\sum_{r=0}^{\frac{1}{2}N-1} y_{2r+1} \exp\left(-i\frac{2\pi k(2r+1)}{N}\right) =$$

$$e^{-i2\pi k/N} \sum_{r=0}^{\frac{1}{2}N-1} y_{2r+1} \exp\left(-i\frac{2\pi kr}{N/2}\right) = e^{-i2\pi k/N} O_k$$

→ again a DFT with N/2 points, times a phase factor.

  - We now can do the DFT in $2(N/2)^2$ operations!

Fast Fourier Transform (FFT)

- So, we halved the number of operations to do!

$$c_k = E_k + e^{-i2\pi k/N} O_k$$

- But why stop here? Do this again for each of the DFTs, and again, … until we are left with just a single point (whose transform is the point itself). Can do this because there are 2^m points in total.

- How many operations we need to do now?

  → $N\log_2 N$ – way better than the original N^2!

  e.g. for $N\log_2 N=10^9$ we have N~40 million.

- Even 2D and 3D FTs become feasible now. FFTs can be done also for non-2^m sizes (but algebra is quite tedious).

DFTs and FFTs in Python

- Provided by module numpy.fft
- Includes a variety of functions (check help),

  e.g. rfft → 1D real DFT (using FFT)

  irfft → inverse of rfft

  fftpack.ffn → N-dimensional DFT (using FFT)

- Sample usage:

```
from numpy import array
y=array([0.,0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9],float)   ← input data
c=rfft(y)                                                  ← forward FFT
print(c)
[ 4.5+0.j         -0.5+1.53884177j   -0.5+0.68819096j   -0.5+0.36327126j
  -0.5+0.16245985j   -0.5+0.j         ]          ← Fourier coefficients (why only 6?)
y1=irfft(c)                                                ← inverse FFT
print(y1)
[ 0.   0.1  0.2  0.3  0.4  0.5  0.6  0.7  0.8  0.9]
```