MAS212 Scientific Computing and Simulation

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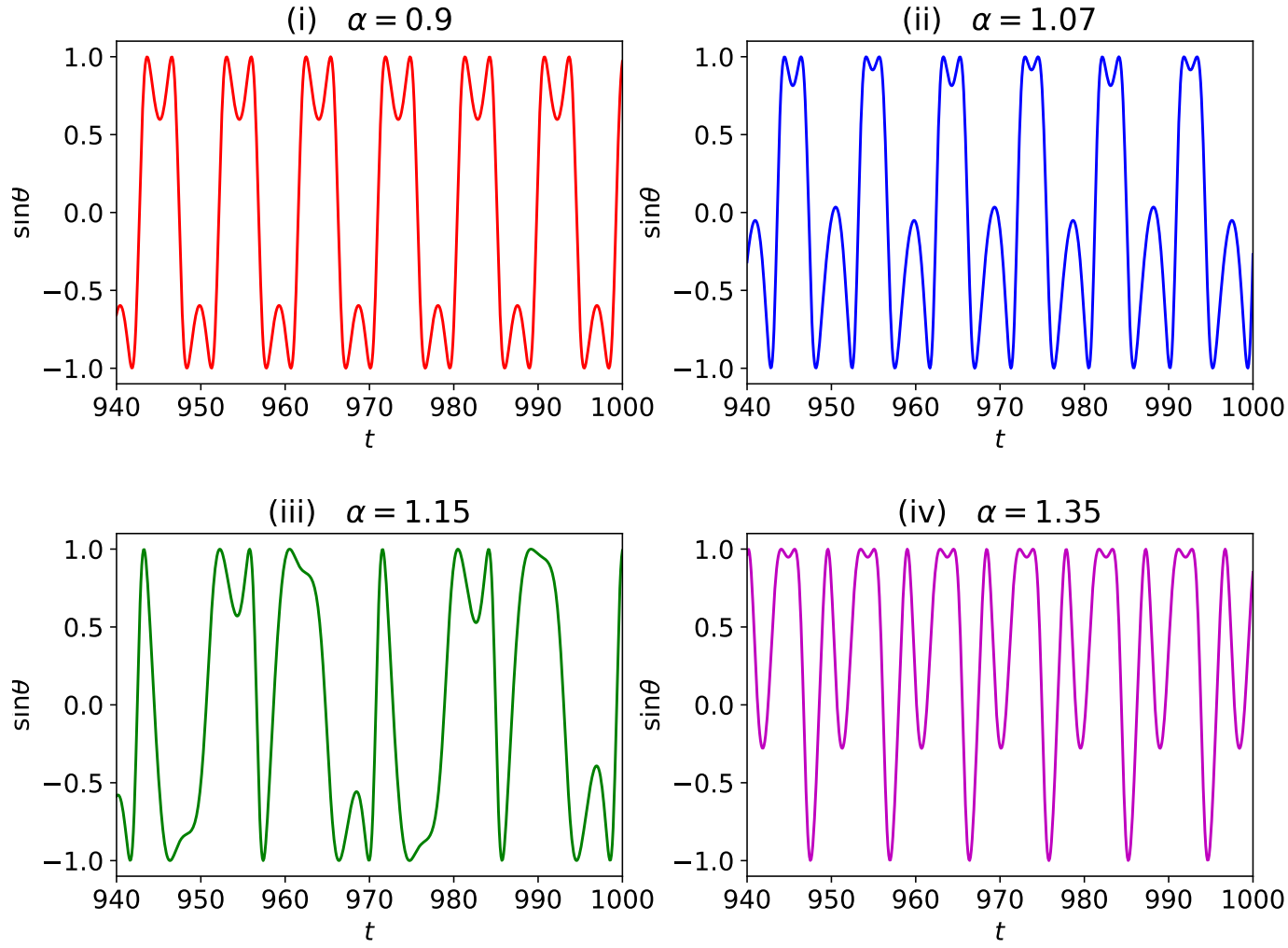
Today's lecture

- The **Discrete Fourier Transform** (DFT)
- **Motivations:**
  - finding the frequencies in the damped driven oscillator
  - looking for hidden signals in experimental data
- Definition of DFT and 3 examples
- The inverse DFT
- DFT and **Fourier series**
- **Example:** Gibbs' phenomenon
- Filtering

Motivation (1): Damped driven oscillator

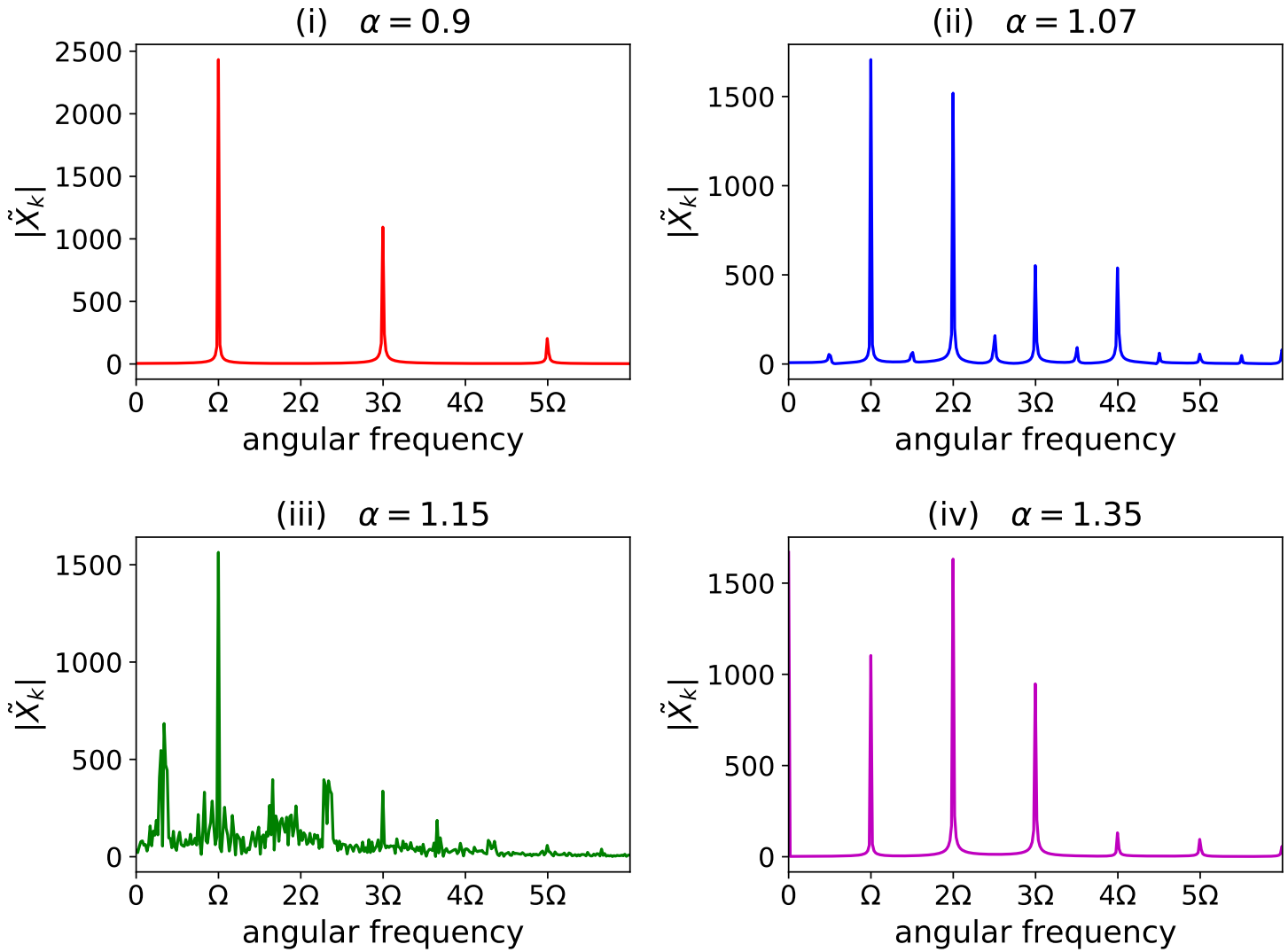


- Assignment 2 asked: Is the response periodic? What is the fundamental period?

Motivation (1): The damped driven oscillator

. . . now take the Discrete Fourier Transform . . .

Motivation (1): The damped driven oscillator



- The DFT reveals the harmonics present in the signal.

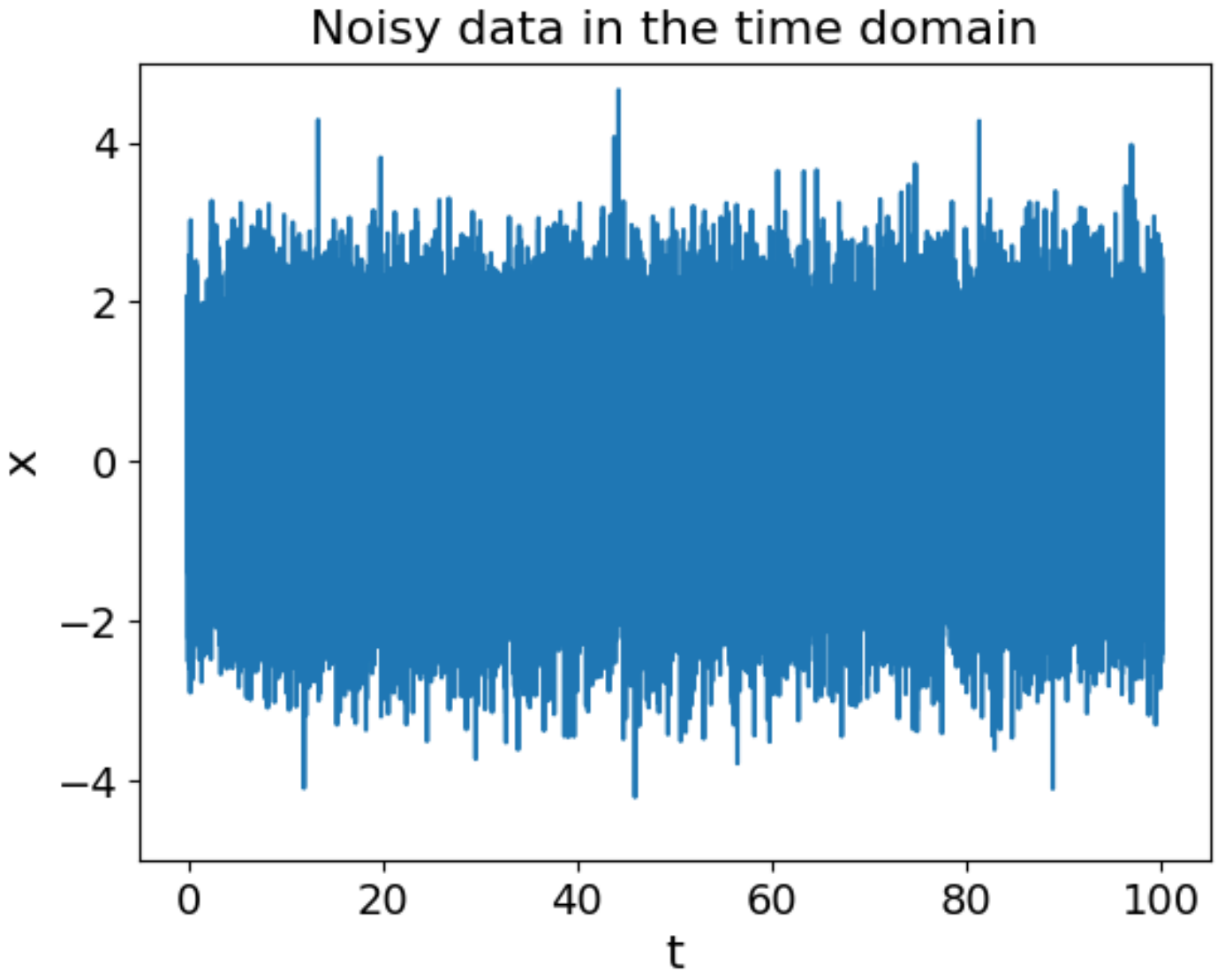
Motivation (2)

- **Toy Model:** Imagine a scientific instrument (e.g. a seismometer or radio telescope) measuring noisy data with a hidden signal.
- For example,

$$y(t) = 0.1\sin(3t) + 0.06\cos(7t) + n(t)$$

- Here blue = signal and red = noise.
- Suppose $n(t)$ is noise from a Gaussian distribution with standard deviation $\sigma = 1$.

Motivation (2): Noisy data with hidden signal

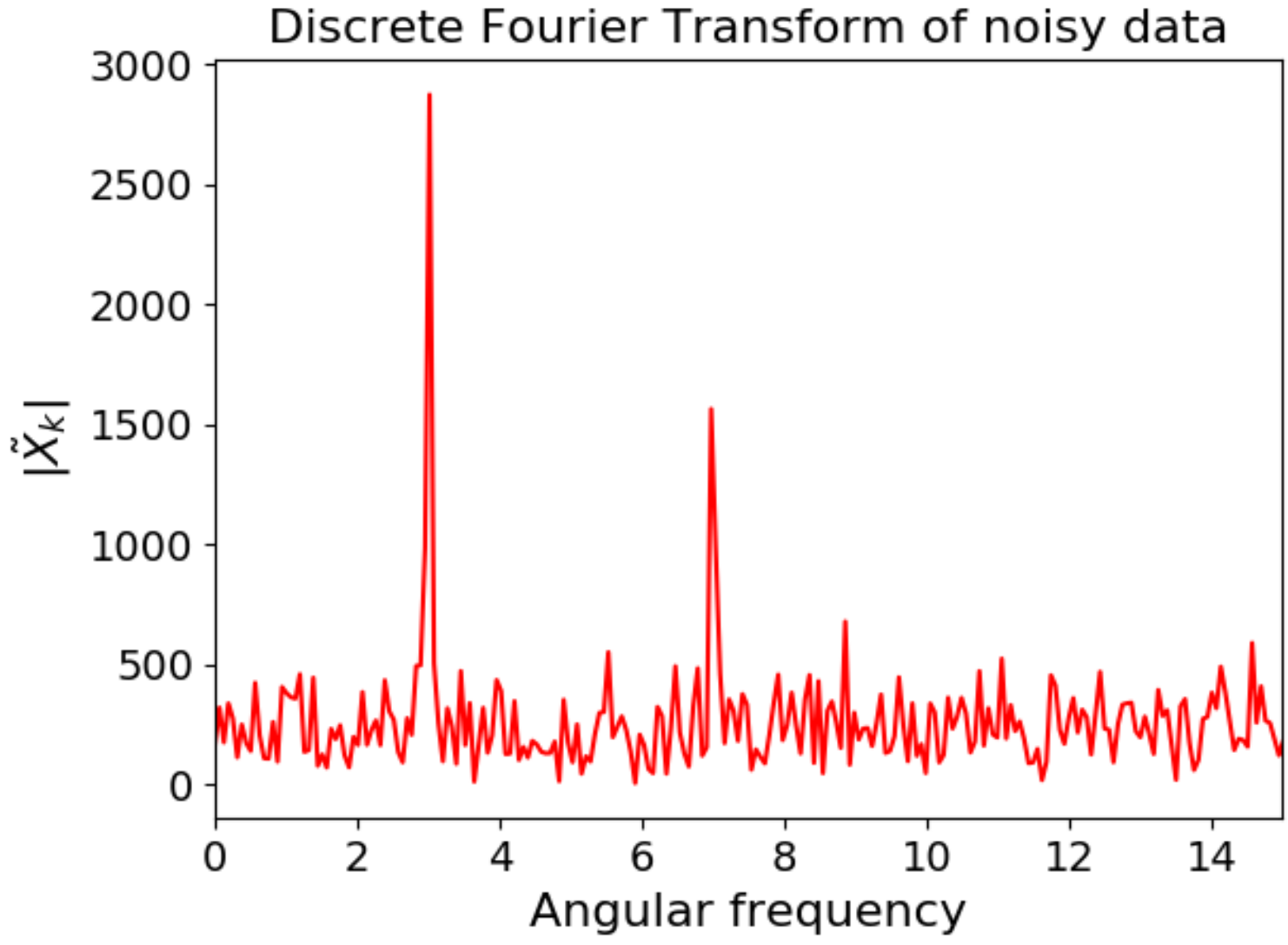


(a) time domain: nothing visible

Motivation (2): Noisy data with hidden signal

. . . now take the Discrete Fourier Transform . . .

Motivation (2): Noisy data with hidden signal



(b) frequency domain: two ‘spikes’.

Code for this example

Generating the noisy data:

```
n = 2**15
tmax = 100
ts = np.linspace(0,tmax,n)
h = ts[1]-ts[0]
ys = 0.1*np.sin(3*ts) + 0.06*np.cos(7.0*ts) +
                                    np.random.normal(size=n)
plot(ts, ys, 'b-')
```

Taking the Discrete Fourier Transform:

```
zs = np.fft.fft(ys)
ws = np.fft.fftfreq(ts.size, h)
plt.plot(2.0*np.pi*ws, zs.real**2 + zs.imag**2, 'r-')
plt.xlim(0, 15)
```

The Discrete Fourier Transform (DFT)

Definition:

- Suppose we have a data set made up of a sequence of complex numbers: $x_0, x_1, \ldots x_{n-1}$
- The discrete Fourier transform (DFT) of x_j is the sequence of **complex numbers** $\tilde{X}_k$ defined by

$$\tilde{X}_k \equiv \sum_{j=0}^{n-1} x_j \exp\left(-i\,2\pi jk/n\right), \qquad j,k \in \mathbb{Z},$$

  where i is the unit imaginary.
- The sequence $\tilde{X}_k$ is ***n*-periodic** (as $e^{2i\pi} = 1$):

$$\tilde{X}_{k\pm n} = \tilde{X}_k$$

- $\tilde{X}_k$ are called the **Fourier coefficients** of x_j.

The Discrete Fourier Transform (DFT)

Examples:

Consider the following sequences x_j,
where $n = 100$ and $j = 0, 1, \ldots, n-1$ and $t_j = j/n$:

(a) $x_j = \sin(10\pi t_j) + \frac{1}{2}\cos(20\pi t_j)$

(b) $x_j = t_j^2$.

(c) $x_j = \exp\left(-200\left(t_j - \frac{1}{2}\right)^2\right)$

1. Plot these sequences.
2. Compute the Fourier coefficients $\tilde{X}_k$ and plot.

Solution:

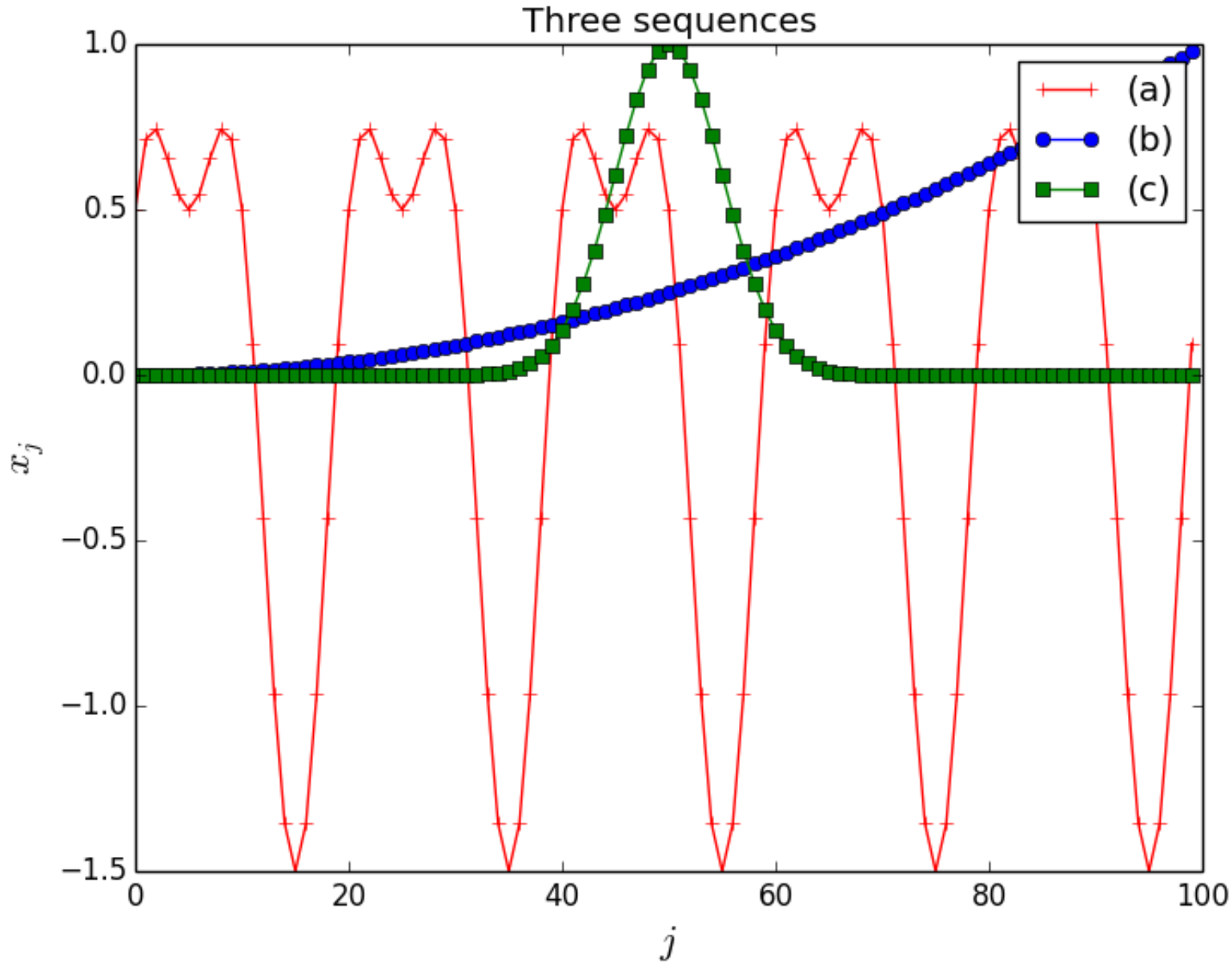
(1) Generate the sequences and plot:

```
import numpy as np
import matplotlib.pyplot as plt
```

```
n = 100
js = np.arange(n)
ts = js / float(n)
x_a = np.sin(10*np.pi*ts) + 0.5*np.cos(20*np.pi*ts)
x_b = ts**2
x_c = np.exp(-200*(ts-0.5)**2)
```

```
plt.plot(js, x_a, 'r+-', label='(a)')
plt.plot(js, x_b, 'bo-', label='(b)')
plt.plot(js, x_c, 'gs-', label='(c)')
```

Solution (1):



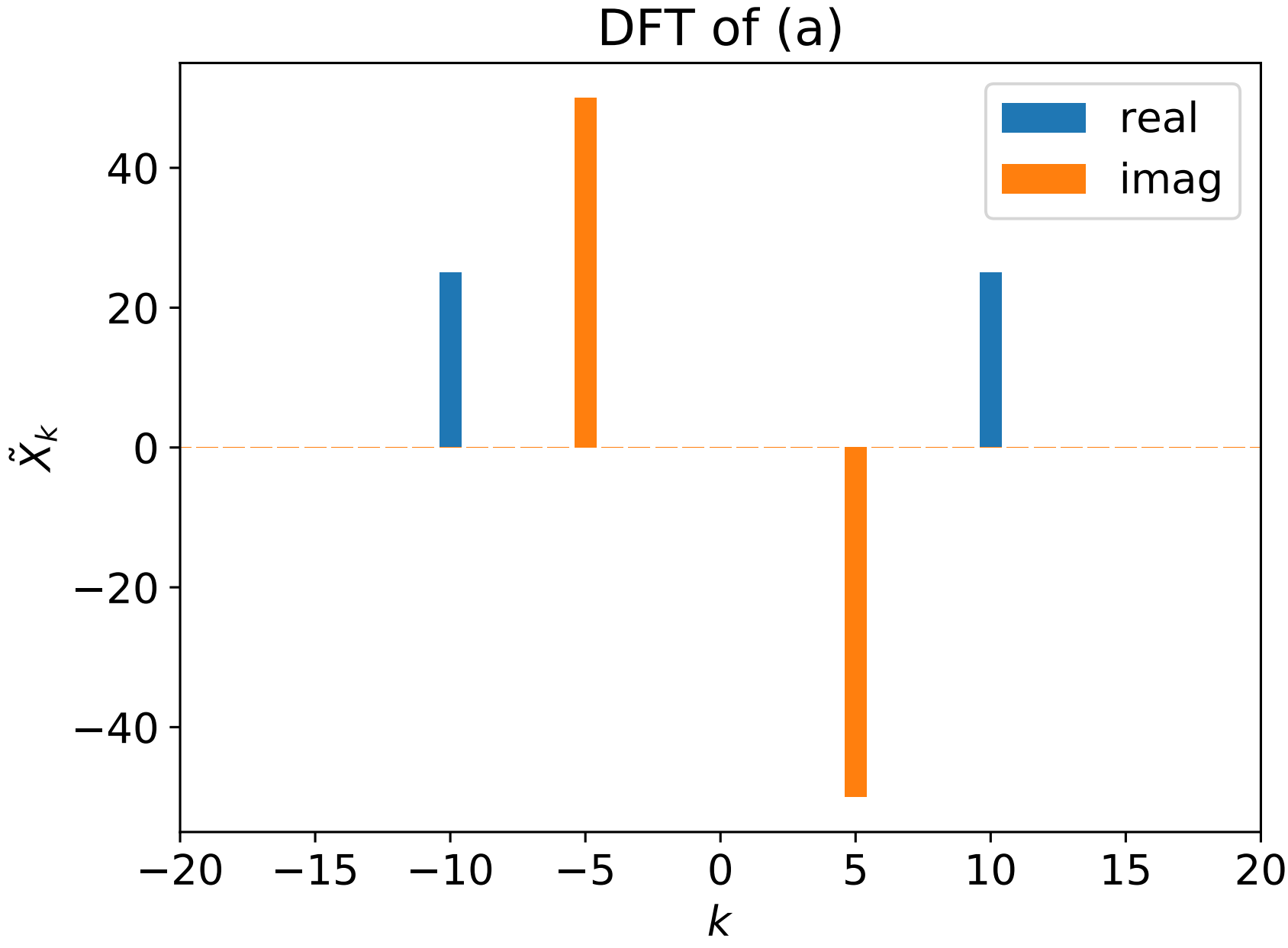
Solution (2):

- Python has **two** modules for DFTs:
  `numpy.fft` and `scipy.fftpack`.
- FFT = **Fast** Fourier Transform (efficient algorithm).
- Remember that $\tilde{X}_k$ are **complex numbers**.
- We want to plot $\tilde{X}_k$ **symmetrically** about $k = 0$.

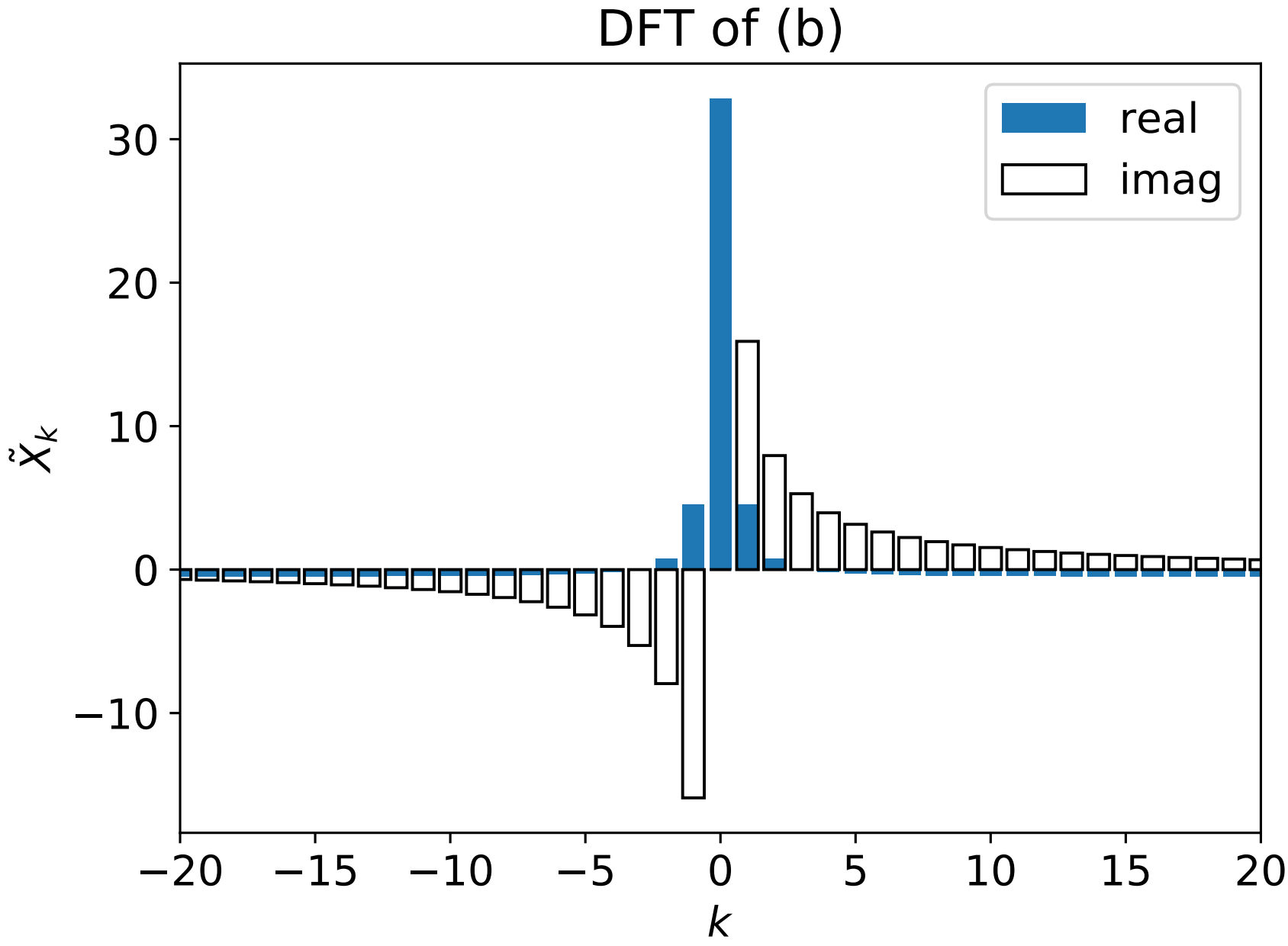
```
Xt_a = np.fft.fft(x_a)     # compute the DFT
ks = np.fft.fftfreq(n, d=1.0/n) # get the array of k values
plt.plot(ks, Xt_a.real, 'r+', label='real')
plt.plot(ks, Xt_a.imag, 'b+', label='imag')
plt.legend()
plt.show()
```

- For real x_j, the DFT is **Hermitian**: $X_{-k} = X_k^*$.

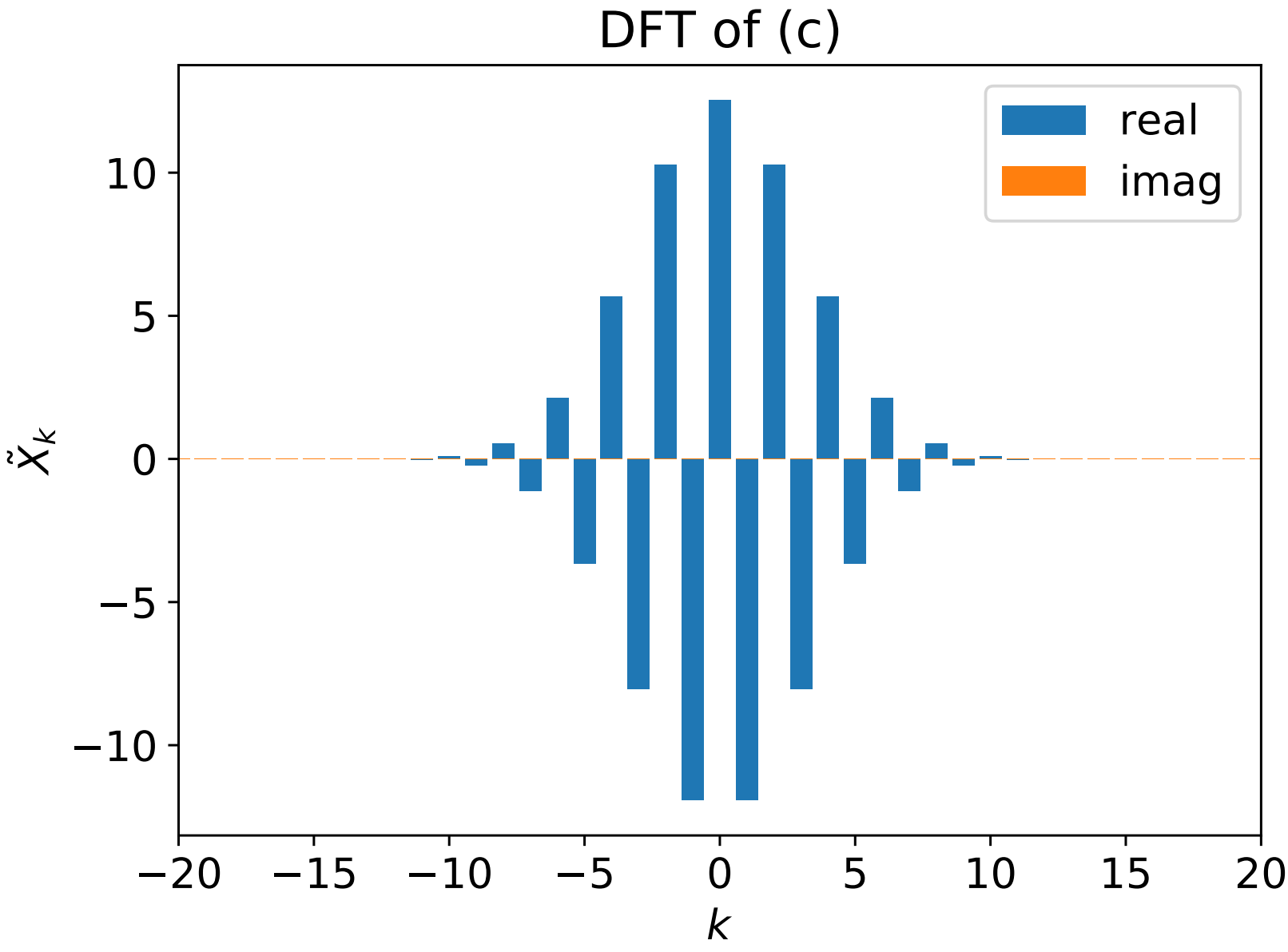
(a) $x_j = \sin(10\pi t_j) + \frac{1}{2}\cos(20\pi t_j)$



(b) $x_j = t_j^2$



(c) $x_j = \exp\left(-200\left(t_j - \frac{1}{2}\right)^2\right)$



The Inverse Transform

Inverse Discrete Fourier Transform

- The inverse DFT **goes the other way**:

$$x_j = \frac{1}{n} \sum_{k=0}^{n-1} \tilde{X}_k \exp\left(+i\,2\pi jk/n\right)$$

- Compare with

$$\tilde{X}_k \equiv \sum_{j=0}^{n-1} x_j \exp\left(-i\,2\pi jk/n\right)$$

- For the inverse transformation, use `numpy.fft.ifft()`.

Proof of inverse formula:

- Substitute definition of $\tilde{X}_k$ into inverse formula:

$$
\begin{aligned}
& \frac{1}{n} \sum_{k=0}^{n-1} \left\{ \tilde{X}_k \right\} \exp\left(+i\, 2\pi jk/n\right) \\
= \quad & \frac{1}{n} \sum_{k=0}^{n-1} \left\{ \sum_{j'=0}^{n-1} x_{j'} \exp\left(-i\, 2\pi j' k/n\right) \right\} \exp\left(+i\, 2\pi jk/n\right) \\
= \quad & \sum_{j'=0}^{n-1} x_{j'} \times \frac{1}{n} \sum_{k=0}^{n-1} \exp\left(+i\, 2\pi (j-j')k/n\right) \\
= \quad & \sum_{j'=0}^{n-1} x_{j'} \delta_{jj'} \\
= \quad & x_j \qquad \text{as required.}
\end{aligned}
$$

- N.B. $\delta_{jj'}$ is 1 if $j' = j$, and 0 otherwise.

Summary:

$$x_j = \frac{1}{n} \sum_{k=0}^{n-1} \tilde{X}_k e^{+i\,2\pi jk/n} \qquad \Leftrightarrow \qquad \tilde{X}_k \equiv \sum_{j=0}^{n-1} x_j e^{-i\,2\pi jk/n}$$

Interpreting the DFT

- Suppose $\{x_j\}$ is a data set of length n, sampled at regular time intervals Δt:

$$t_j \equiv j\Delta t.$$

- We can think of the DFT as a map from the 'time domain' to the 'frequency domain':

$$(t_j, x_j) \longrightarrow (\omega_k, \tilde{X}_k)$$

where

$$\omega_k = k\Delta\omega, \qquad \Delta\omega = \frac{2\pi}{n\Delta t},$$

such that $2\pi jk/n = \omega_k t_j$.

- The frequency interval $\Delta\omega$ is inversely proportional to the total duration $n\Delta t$.

- The maximum frequency ($\omega_{\text{max}} = 2\pi/\Delta t$) is inversely proportional to the sampling interval Δt.

Interpreting the DFT

Suppose x_j are **real** measurements at times $t_j = j\Delta t$.

- x_j are real $\Leftrightarrow$ $\tilde{X}_k$ are **Hermitian**: $\tilde{X}_k^* = \tilde{X}_{-k}$
- $\Rightarrow$ $\tilde{X}_0$ is **real**: $\tilde{X}_0 = \sum x_j = n\bar{x}$
- Let $\tilde{X}_k = a_k - ib_k$. Then

$$x_j = \frac{1}{2}a_0 + \frac{2}{n}\sum_{k=1}^{n-1}\left\{a_k \cos\left(\omega_k t_j\right) + b_k \sin\left(\omega_k t_j\right)\right\}$$

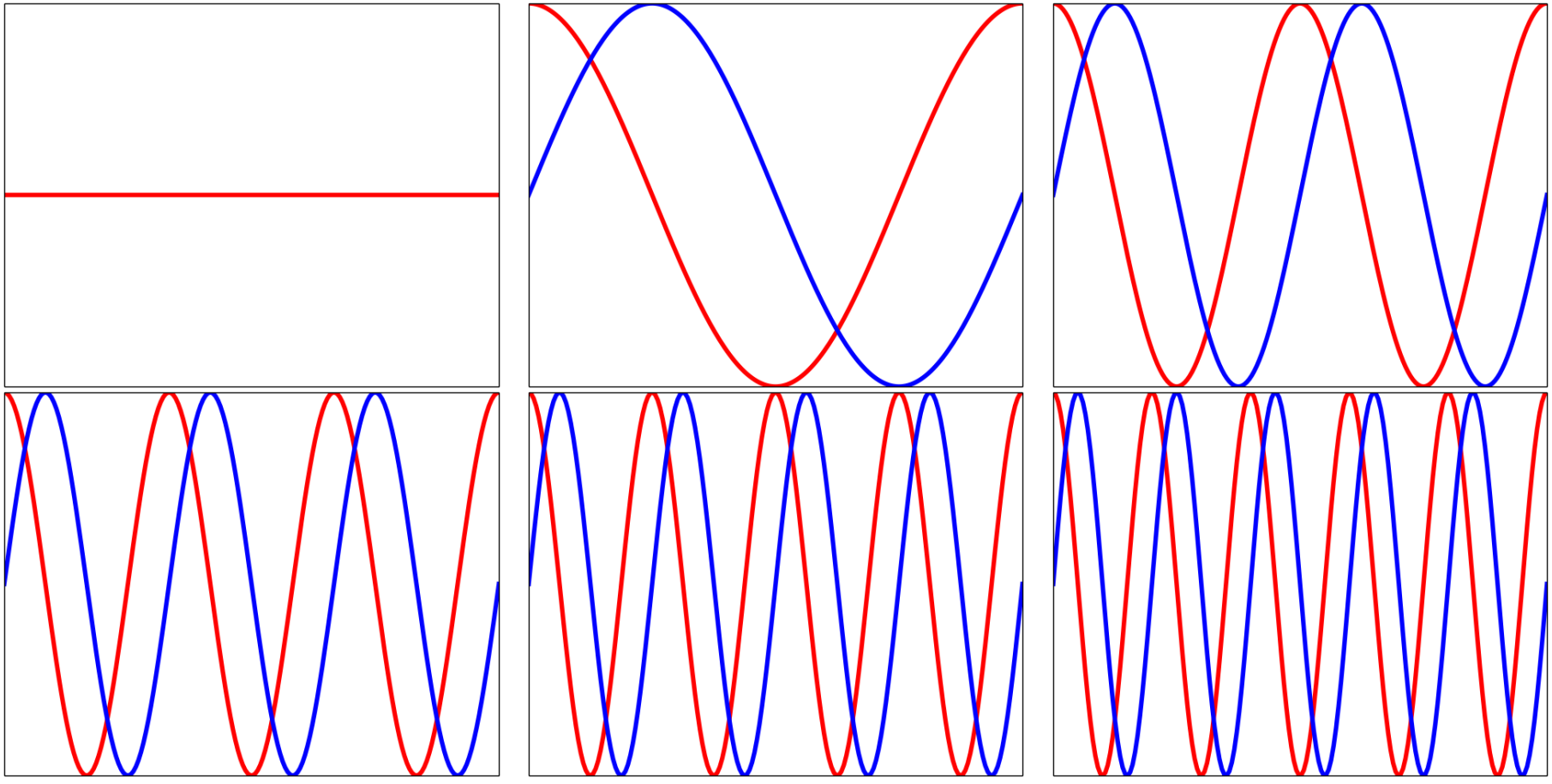
where a_k and b_k are real coefficients

$$a_k = \text{Re}\sum_{j=0}^{n-1} x_j e^{-i\,2\pi jk/n} = \sum_{j=0}^{n-1} x_j \cos\left(\omega_k t_j\right)$$

$$b_k = -\text{Im}\sum_{j=0}^{n-1} x_j e^{-i\,2\pi jk/n} = \sum_{j=0}^{n-1} x_j \sin\left(\omega_k t_j\right)$$

Interpreting the DFT

- x_j is made up of a sum of harmonics:
- a_k and b_k are the amplitudes of the harmonics



Fourier series

- The **Fourier series expansion** of a real function $x(t)$ in the domain $t_0 \leq t < t_0 + T$ is:

$$x(t) = \frac{1}{2}a_0 + \sum_{k=1}^{\infty} \{a_k \cos(\omega_k t) + b_k \sin(\omega_k t)\}.$$

where $\omega_k = \dfrac{2\pi k}{T}$.

- The Fourier coefficients a_k and b_k are:

$$\begin{aligned} a_k &= \frac{2}{T}\int_{t_0}^{t_0+T} x(t)\cos(\omega_k t)dx \\ b_k &= \frac{2}{T}\int_{t_0}^{t_0+T} x(t)\sin(\omega_k t)dx. \end{aligned}$$

Example:

Consider the **'step function'**:

$$x(t) = \begin{cases} 1, & t \geq 0, \\ 0, & t < 0, \end{cases}$$

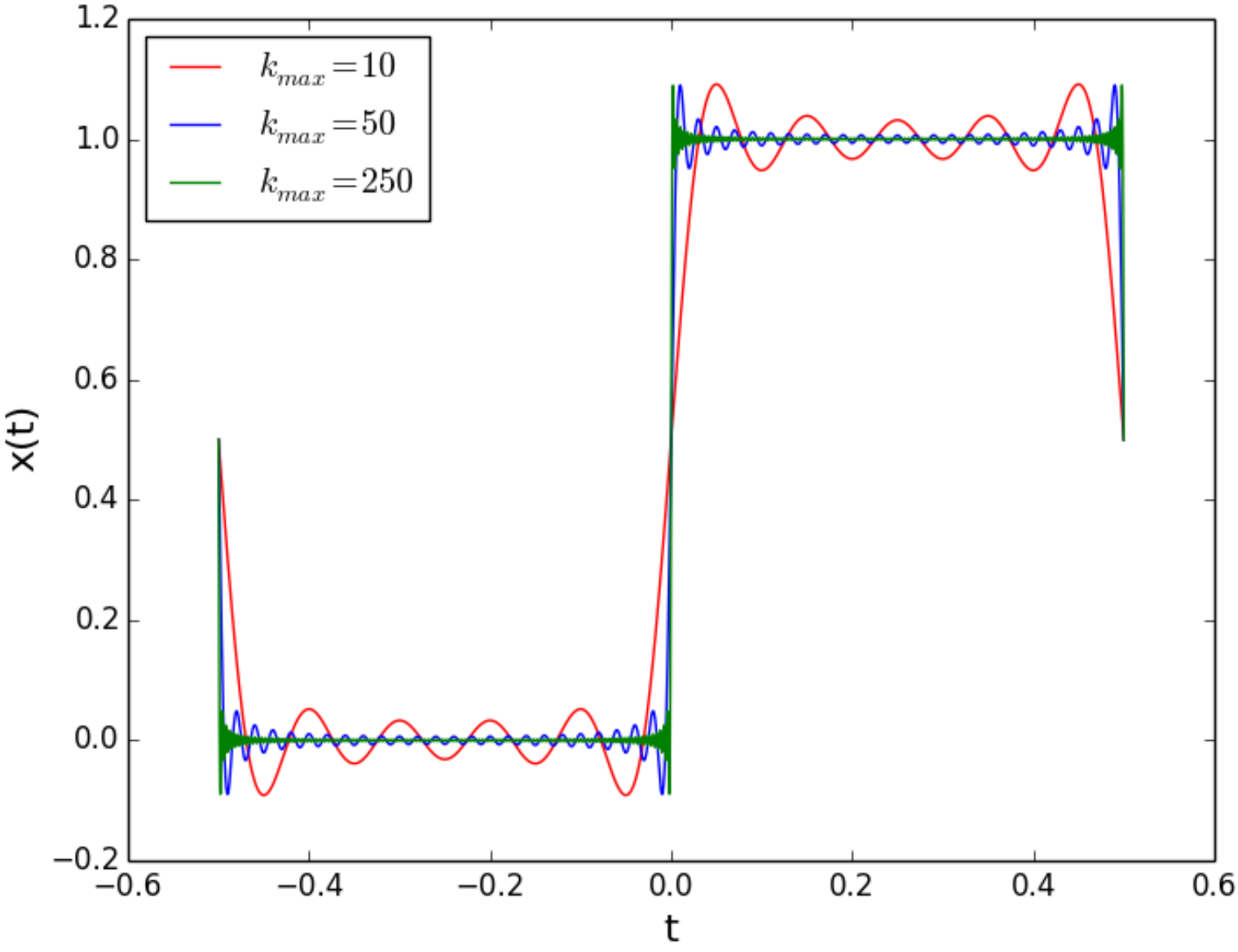
on the domain $-T/2 \leq t \leq T/2$.

(a) Show that the Fourier representation of $x(t)$ is

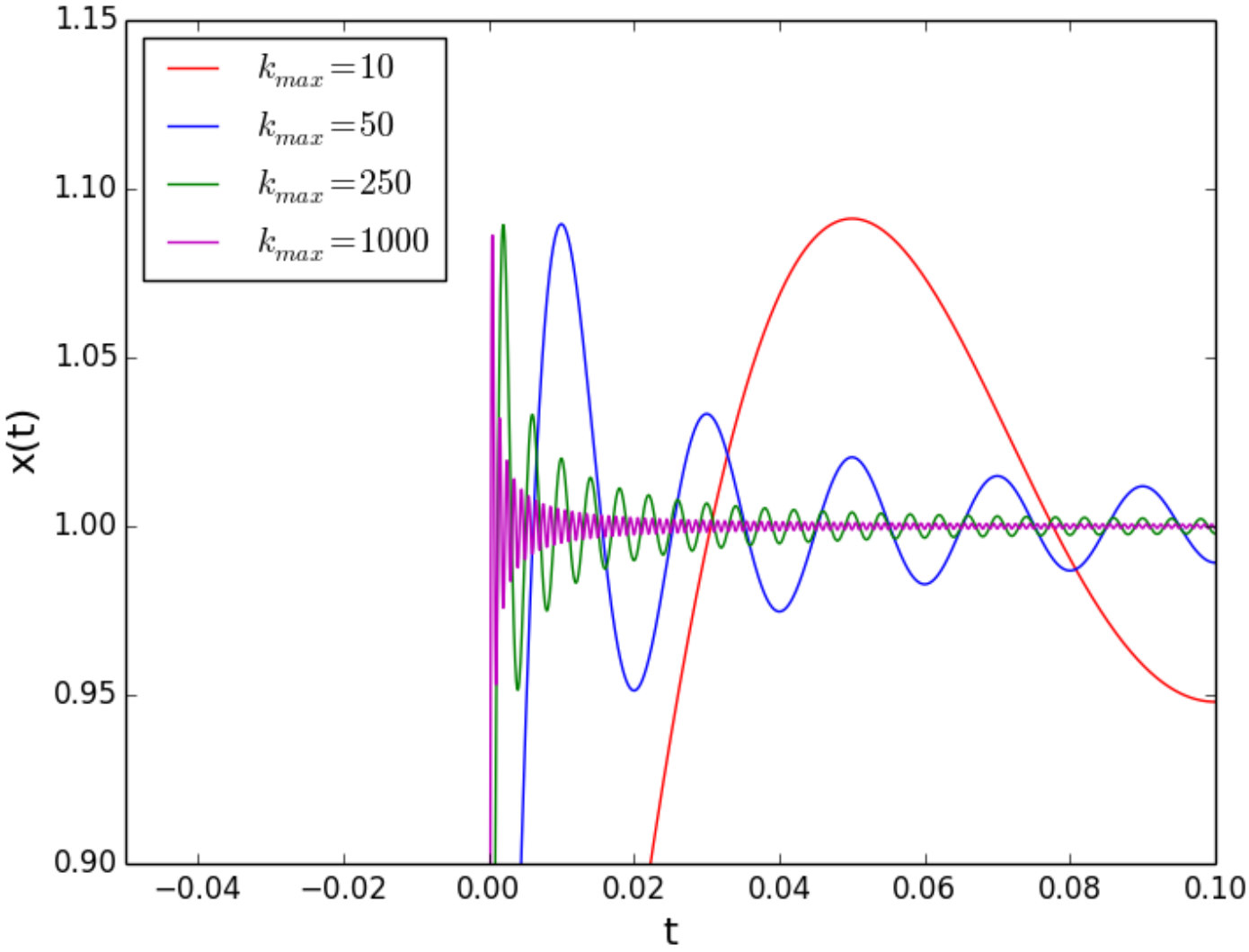
$$\frac{1}{2} + \sum_{k \text{ odd}}^{\infty} \left(\frac{2}{\pi k} \right) \sin(\omega_k t).$$

(b) Set $T = 1$ and compute the Fourier sum up to (i) $k = 10$, (ii) $k = 50$, (iii) $k = 250$. What do you notice?

Solution:


$k_{max}=10$
$k_{max}=50$
$k_{max}=250$
x(t)
t
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6

Solution:



- The overshoot of $\sim 9\%$ **does not disappear** as $k_{\text{max}} \to 0$.

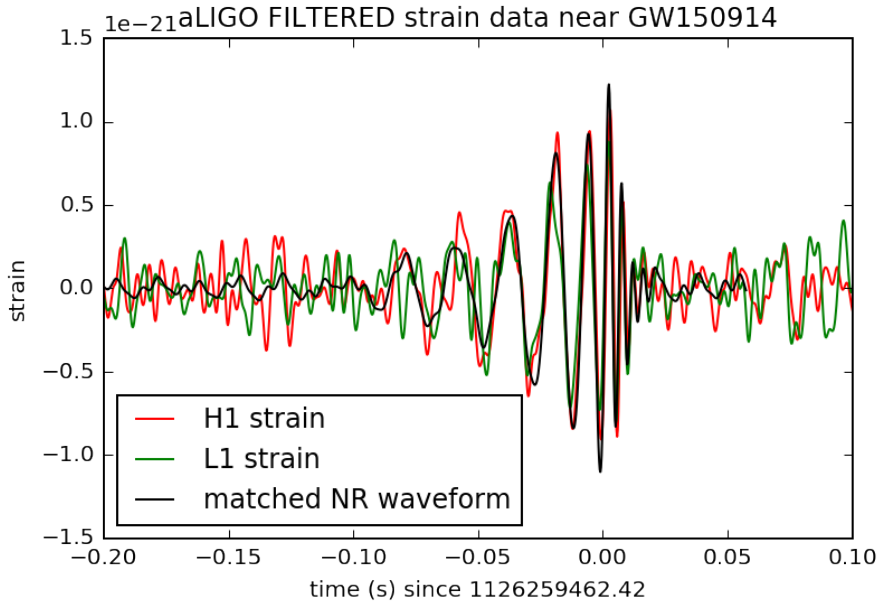
Gibbs' Phenomenon

If $x(t)$ is a function with discontinuities:

- Its Fourier series will overshoot at each discontinuity
- The overshoot will **not** disappear as the number of terms in the sum increases.

Filtering

- Many signal processing algorithms work as follows:
  - Apply a DFT
  - Apply a filter (e.g. remove high or low frequencies)
  - Apply an inverse DFT.
- **Example:** For a tutorial in signal processing for **gravitational-wave detectors**, see `https://losc.ligo.org/s/events/GW150914/GW150914_tutorial.ipynb`



Filtering

- Suppose I wanted to use a **low-pass filter** to remove the high frequencies from a data set a_j.
- I can define a **filter** in terms of its Fourier components $\tilde{F}_k$,
- then define a **filtered dataset** b_j via

$$b_j = IDFT(\tilde{B}_k), \qquad \tilde{B}_k = \tilde{A}_k \tilde{F}_k$$

- A naive low-pass filter would be:

$$\tilde{F}_k = \Theta(k, k_0) \equiv \begin{cases} 0 & |k| > k_0 \\ 1 & \text{otherwise} \end{cases}, \quad -\frac{n}{2} \leq k \leq \frac{n}{2}.$$

- But this is not suitable. **Why not**? First we need to understand the **convolution theorem**.

Convolution

Definition:

- The convolution of two n-periodic sequences a_j and b_j is defined by

$$(a \otimes b)_j = \sum_{j'=0}^{n-1} a_{j'} b_{j-j'}$$

Notes:

- Convolution is like **smearing** one sequence with another.

The Convolution Theorem

- Suppose a_j and b_j are sequences with Fourier coefficients $\tilde{A}_k$ and $\tilde{B}_k$. Now consider the sequence c_j whose Fourier coefficients are $\tilde{C}_k = \tilde{A}_k \tilde{B}_k$. What are c_j?

$$
\begin{aligned}
c_j &= \frac{1}{n} \sum_{k=0}^{n-1} \left(\tilde{A}_k \tilde{B}_k \right) \exp\left(i\, 2\pi jk/n \right) \\
&= \frac{1}{n} \sum_k \sum_p \sum_q a_p e^{-i2\pi pk/n} b_q e^{-i2\pi qk/n} e^{i2\pi jk/n} \\
&= \sum_p \sum_q a_p b_q \times \frac{1}{n} \sum_k \exp\left(i \frac{2\pi k}{n} (j - p - q) \right) \\
&= \sum_p a_p b_{j-p} = (a \otimes b)_j
\end{aligned}
$$

- That is, c_j is the **convolution** of a_j and b_j.

The Convolution Theorem

- This works both ways:

$$\tilde{C}_k = \tilde{A}_k \tilde{B}_k \qquad \Leftrightarrow \qquad c_j = (a \otimes b)_j$$

and

$$\tilde{C}_k = \left(\tilde{A} \otimes \tilde{B}\right)_k \qquad \Leftrightarrow \qquad c_j = a_j b_j.$$

Practical application

- Naive low-pass filter:

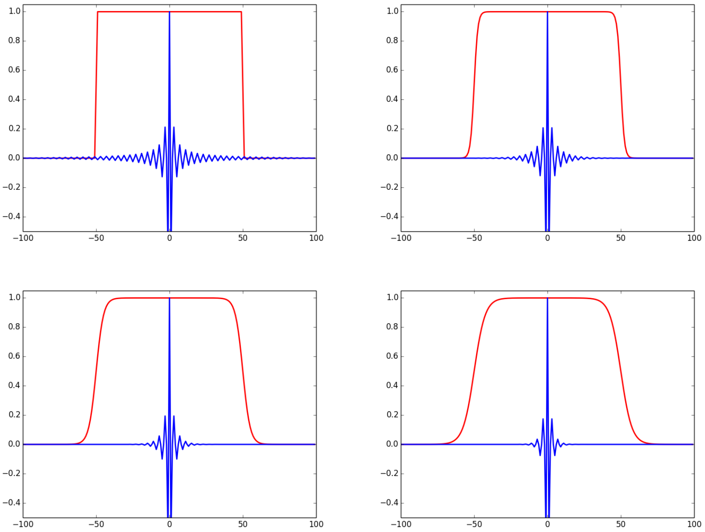
$$\tilde{F}_k = \Theta(k, k_0) \equiv \begin{cases} 0 & |k| > k_0 \\ 1 & \text{otherwise} \end{cases} \quad \text{for} \quad -\frac{n}{2} \leq k \leq \frac{n}{2}.$$

- Defining $c = \pi j/n$,

$$\begin{aligned} f_j &= \frac{1}{n} \sum_{k=-n/2}^{n/2-1} \Theta(k, k_0) e^{2ick} \\ &= \frac{1}{n} \sum_{k=-k_0}^{k_0} \left(e^{2ic}\right)^k \\ &= \frac{1}{n} \frac{e^{ic(2k_0+1)} - e^{-ic(2k_0+1)}}{e^{ic} - e^{-ic}} \\ &= \frac{1}{n} \frac{\sin((2k_0+1)\pi j/n)}{\sin(\pi j/n)} \end{aligned}$$

- This is **wide** and oscillatory. Not suitable.

Filters and their Inverse DFTs



Red = filter in frequency domain,   Blue = time domain profile.