Senior Fresh Computational Physics Laboratory Report

# Laboratory 4: Fourier Analysis

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## Contents

# 1 Introduction

The aim of this laboratory was to investigate Fourier analysis by computing Fourier series and transforms for various functions.

## 1.1 Simpson's Rule

There are many numerical methods to integrate a function on some bounds. One such approach is Simpson's rule. The idea behind this method is to approximate the function as a parabola over each interval on the bounds.

The integral of a quadratic function $f(x) = Ax^2 + Bx + C$ from $-h$ to $h$ can be expressed in terms of the value of the function at $-h$, 0, and $h$ as

$$\begin{aligned}
\int_{-h}^{h} \left(Ax^2 + Bx + C\right) dx &= \frac{Ax^3}{3} + \frac{Bx^2}{2} + Cx + D\bigg|_{-h}^{h} \\
&= \frac{2Ah^3}{3} + 2Ch \\
&= \frac{h}{3}\left(\left(Ah^2 - Bh + C\right) + 4C + \left(Ah^2 + Bh + C\right)\right) \\
&= \frac{h}{3}\left(f(-h) + 4f(0) + f(h)\right). \qquad (1)
\end{aligned}$$

The integral over the adjacent interval of length $2h$, from $h$ to $3h$, can similarly be found as

$$\begin{aligned}
\int_{h}^{3h} \left(Ax^2 + Bx + C\right) dx &= \frac{Ax^3}{3} + \frac{Bx^2}{2} + Cx + D\bigg|_{h}^{3h} \\
&= \frac{26Ah^3}{3} + 4Bh^2 + 2Ch \\
&= \frac{h}{3}\left(\left(Ah^2 + Bh + C\right) + 4\left(4Ah^2 + 2Bh + C\right) + \left(9Ah^2 + 3Bh + C\right)\right) \\
&= \frac{h}{3}\left(f(h) + 4f(2h) + f(3h)\right). \qquad (2)
\end{aligned}$$

Combining equations (1) and (2) leads to the following expression for the integral from $-h$ to $3h$:

$$\begin{aligned}
\int_{-h}^{3h} \left(Ax^2 + Bx + C\right) dx &= \int_{-h}^{h} \left(Ax^2 + Bx + C\right) dx + \int_{h}^{3h} \left(Ax^2 + Bx + C\right) dx \\
&= \frac{h}{3}\left(f(-h) + 4f(0) + f(h)\right) + \frac{h}{3}\left(f(h) + 4f(2h) + f(3h)\right) \\
&= \frac{h}{3}\left(f(-h) + 4f(0) + 2f(h) + 4f(2h) + f(3h)\right). \qquad (3)
\end{aligned}$$

Equation (3) can be expanded to any number of intervals of length $2h$ in a similar fashion. Simpson's rule utilises this by approximating the function to be integrated $f$ as a parabola over $n$ equally spaced intervals of length $2h$, and repeating the method outlined above. This results in

$$\int_a^b f(x)\, dx \approx \frac{h}{3}\left(f(a) + 2\sum_{i=1}^{\frac{n}{2}-1} f(a + 2jh) + 4\sum_{i=1}^{\frac{n}{2}} f(a + 2jh - 1) + f(b)\right), \qquad (4)$$

where $n$ is an even number, and $h \equiv \frac{b-a}{n}$.

## 1.2 Fourier Series for Periodic Functions

In 1807, Joseph Fourier discovered that any periodic function can be written as an infinite sum of harmonic functions.[1] A function $f$ of period $T = \frac{2\pi}{\omega}$ can be written as

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left( a_n \cos(n\omega t) + b_n \sin(n\omega t) \right), \tag{5}$$

where the Fourier coefficients are given by

$$a_k = \frac{2}{T} \int_0^T f(t) \cos(k\omega t)\, dt \tag{6}$$

$$b_k = \frac{2}{T} \int_0^T f(t) \sin(k\omega t)\, dt. \tag{7}$$

In theory, the integral bounds in equations (6) and (7) can be over any interval of length $T$, but it is often more convenient to set the lower bound to 0.

For rectangular wave functions $f(\omega t) = 1$ if $0 \leqslant \omega t < \omega\tau$, and $f(\omega t) = -1$ if $\omega\tau \leqslant \omega t < 2\pi$, the analytic values of the Fourier coefficients are[2]

$$a_0 = \frac{2}{\alpha} - 1 \tag{8}$$

$$a_k = \frac{2}{k\pi} \sin\left(\frac{2k\pi}{\alpha}\right), \quad k \neq 0 \tag{9}$$

$$b_k = \frac{2}{k\pi} \left(1 - \cos\left(\frac{2k\pi}{\alpha}\right)\right), \tag{10}$$

where $\alpha \equiv \frac{2\pi}{\omega\tau}$.

## 1.3 Fourier Transform for Non-Periodic Functions

Although the expansion in equation (5) is for periodic functions, non-periodic functions can also be expressed in terms of sinusoidal functions. Instead of considering a sum over discrete frequencies $k\omega$, the Fourier transform of a non-periodic function concerns an integral over a continuous range of frequencies. This is achieved by taking the limit of equations (5) - (7) as the period $T$ goes to 0, resulting in

$$f(t) = \int_0^{\infty} \left( a(\omega) \cos(\omega t) + b(\omega) \sin(\omega t) \right) d\omega \tag{11}$$

$$a(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} f(t) \cos(\omega t)\, dt \tag{12}$$

$$b(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} f(t) \sin(\omega t)\, dt. \tag{13}$$

One useful expression in many areas of maths and physics is the Fourier transform, defined as

$$F(\omega) = \int_{-\infty}^{\infty} f(t)\, e^{-i\omega t}\, dt. \tag{14}$$

[1] Fourier, 1807

[2] TCD, 2021

For example, if $f(t)$ has dimensions of energy, then the total power in this signal function at a frequency $\omega$ can be calculated from

$$P(\omega) = |F(\omega)|^2 = \Re\left(F(\omega)\right)^2 + \Im\left(F(\omega)\right)^2. \tag{15}$$

The Fourier transform can also be used to compute the original function $f$ by utilising the so-called back-transform, defined as

$$f(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)\, e^{i\omega t}\, d\omega. \tag{16}$$

## 1.4 Discrete Fourier Transform

Instead of having to compute an integral over infinite bounds, the equations above are often replaced with finite sums over a specified interval, in a method known as the discrete Fourier transform (DFT). An advantage of using the DFT is that the function can be non-periodic, or periodic with unknown period.

In the DFT method, the function $f$ is sampled $N$ times over intervals of length $h$ over $t \in [0, h(N-1)]$. In essence, it is assumed that $f$ has period $\tau = Nh$, and $\tau$ is varied by varying $N$ and $h$. Writing $t_m = mh$, $m = 0, 1, 2, \ldots, N-1$ as the discrete time values at which the function is sampled and $\omega_n = \frac{2\pi n}{Nh}$ as the discrete frequency spectrum, and $f_m = f(t_m)$ and $F_n = F(\omega_n)$ for convenience, equations (14) - (16) can be written as

$$\begin{aligned}
F_n &= \sum_{m=0}^{N-1} f_m \left(\cos\left(\frac{2\pi mn}{N}\right) - i\sin\left(\frac{2\pi mn}{N}\right)\right) && (17)\\
P_n &= \Re(F_n)^2 + \Im(F_n)^2 && (18)\\
f_m &= \frac{1}{N}\sum_{n=0}^{N-1} F_n \left(\cos\left(\frac{2\pi mn}{N}\right) + i\sin\left(\frac{2\pi mn}{N}\right)\right). && (19)
\end{aligned}$$

Not every $F_n$ is independent from each other; namely

$$\begin{aligned}
F_{N-n} &= \sum_{m=0}^{N-1} f_m \left(\cos\left(\frac{2\pi m}{N}(N-n)\right) - i\sin\left(\frac{2\pi m}{N}(N-n)\right)\right)\\
&= \sum_{m=0}^{N-1} f_m \left(\cos\left(2\pi m - \frac{2\pi mn}{N}\right) - i\sin\left(2\pi m - \frac{2\pi mn}{N}\right)\right)\\
&= \sum_{m=0}^{N-1} f_m \left[\cos(2\pi m)\cos\left(\frac{2\pi mn}{N}\right) + \sin(2\pi m)\sin\left(\frac{2\pi mn}{N}\right)\right.\\
&\qquad \left. -i\left(\sin(2\pi m)\cos\left(\frac{2\pi mn}{N}\right) - \cos(2\pi m)\sin\left(\frac{2\pi mn}{N}\right)\right)\right]\\
&= \sum_{m=0}^{N-1} f_m \left(\cos\left(\frac{2\pi mn}{N}\right) + i\sin\left(\frac{2\pi mn}{N}\right)\right)\\
F_{N-n} &= F_n^*. && (20)
\end{aligned}$$

From this arises the Nyquist frequency, named after Harry Nyquist.[3] This frequency corresponds to the highest frequency component $F_{\frac{N}{2}-1}$, where

$$\nu = \frac{\omega_{\frac{N}{2}-1}}{2\pi} = \frac{\frac{N}{2}-1}{Nh} = \frac{1}{2h} - \frac{1}{Nh}. \tag{21}$$

# 2 Methodology

## 2.1 Exercise 1: Fourier Series - Sinusoidal Functions

1. A function was chosen and integrated on some bounds, using equation (4) for Simpson's rule with the following code:

```
def Simpson(f, a, b, n):
    h = (b - a) / n
    evens = odds = 0.
    for j in range(1, n / 2):
        evens += f(a + 2. * j * h)
    for j in range(1, n / 2 + 1):
        odds += f(a + (2. * j - 1.) * h)
    return (h / 3.) * (f(a) + 2. * evens + 4. * odds + f(b))
```

   Here, `f` is the function to be integrated from `a` to `b`, taking `n` intervals.

2. The Fourier series of various functions and the corresponding Fourier coefficients were calculated and plotted using equation (5), where the above code was used to calculate the Fourier coefficients in equations (6) and (7).

## 2.2 Exercise 2: Fourier Series - Square & Rectangular Wave Functions

1. The Fourier series of a square wave function was calculated using equation (5), summing over a specified number of terms, using Simpson's rule as in Exercise 1.
2. Step 1. was repeated for a variety of numbers of terms. These series were plotted on the same graph, along with the original function.
3. Step 2. was repeated for a rectangular wave function.

## 2.3 Exercise 3: Discrete Fourier Transform

1. For a chosen function and values of $N$ and $h$, the Fourier components $F_n$ were plotted using equation (17).
2. Step 1. was repeated for a more ideal value of $h$, keeping $N$ fixed. The back-transform was also calculated and plotted for this new value of $h$, using equation (19).
3. A new function was defined, and the Fourier coefficients, power spectrum and back-transform were plotted for this function, for various values of $h$, keeping $N$ constant.

[3] Wolfram MathWorld, 2021

# 3 Results

## 3.1 Exercise 1: Fourier Series - Sinusoidal Functions

Using Simpson's rule with 8 intervals, the integral of $e^x$ from 0 to 1 was calculated to be 1.71828415, a difference of $2.32 \times 10^{-6}$ to the analytical solution of $e - 1 = 1.71828183$, or a percentage error of 0.00014%. For this exercise, the following functions were considered:

$$f_1(t) = \sin(\omega t) \qquad f_3(t) = \sin(\omega t) + 3\sin(3\omega t) + 5\sin(5\omega t)$$

$$f_2(t) = \cos(\omega t) + 3\cos(2\omega t) - 4\cos(3\omega t) \qquad f_4(t) = \sin(\omega t) + 2\cos(3\omega t) + 3\sin(5\omega t).$$

The following graphs of the Fourier series and corresponding coefficients were plotted, only considering the first 8 terms of the Fourier series:

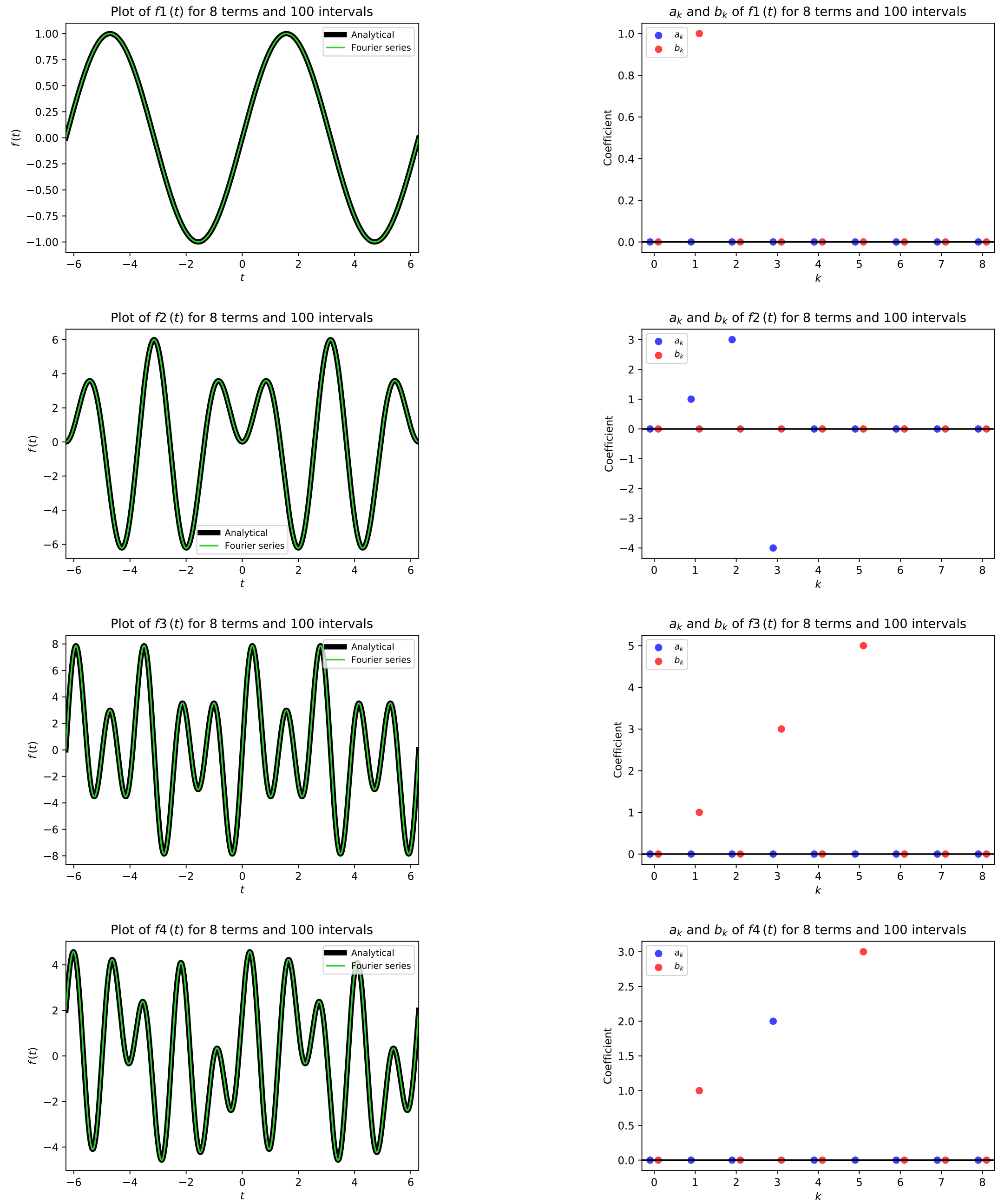



Figure 1: Plots of various periodic functions, their Fourier series, and their Fourier coefficients.

The following values of the Fourier coefficients were calculated for each function:

$$f_1(t) = \sin(\omega t)$$

$|a_k| < 3 \times 10^{-16}$ for all $k$

$b_1 = 1.0000000000000002$
$|b_k| < 2 \times 10^{-16}$ for $k \neq 1$

$$f_2(t) = \cos(\omega t) + 3\cos(2\omega t) - 4\cos(3\omega t)$$

$a_1 = 1.0000000000000004$
$a_2 = 2.999999999999999$
$a_3 = -3.9999999999999996$
$|a_k| < 2 \times 10^{-15}$ for $k \neq 1, 2, 3$

$|b_k| < 2 \times 10^{-15}$ for all $k$

$$f_3(t) = \sin(\omega t) + 3\sin(3\omega t) + 5\sin(5\omega t)$$

$|a_k| < 3 \times 10^{-15}$ for all $k$

$b_1 = 0.9999999999999998$
$b_3 = 3.0000000000000004$
$b_5 = 4.999999999999999$
$|b_k| < 3 \times 10^{-15}$ for $k \neq 1, 3, 5$

$$f_4(t) = \sin(\omega t) + 2\cos(3\omega t) + 3\sin(5\omega t)$$

$a_3 = 1.9999999999999996$
$|a_k| < 7 \times 10^{-16}$ for $k \neq 1$

$b_1 = 0.9999999999999998$
$b_5 = 2.999999999999999$
$|b_k| < 2 \times 10^{-15}$ for $k \neq 1, 5$

Within a reasonable tolerance, these coefficients are the same as those of the original function, and the Fourier series of each function matches the original. This is as expected, as each of these functions is a finite superposition of sinusoidal functions of period $T$, and the Fourier series is simply an infinite sum of all sinusoidal functions of period $T$.

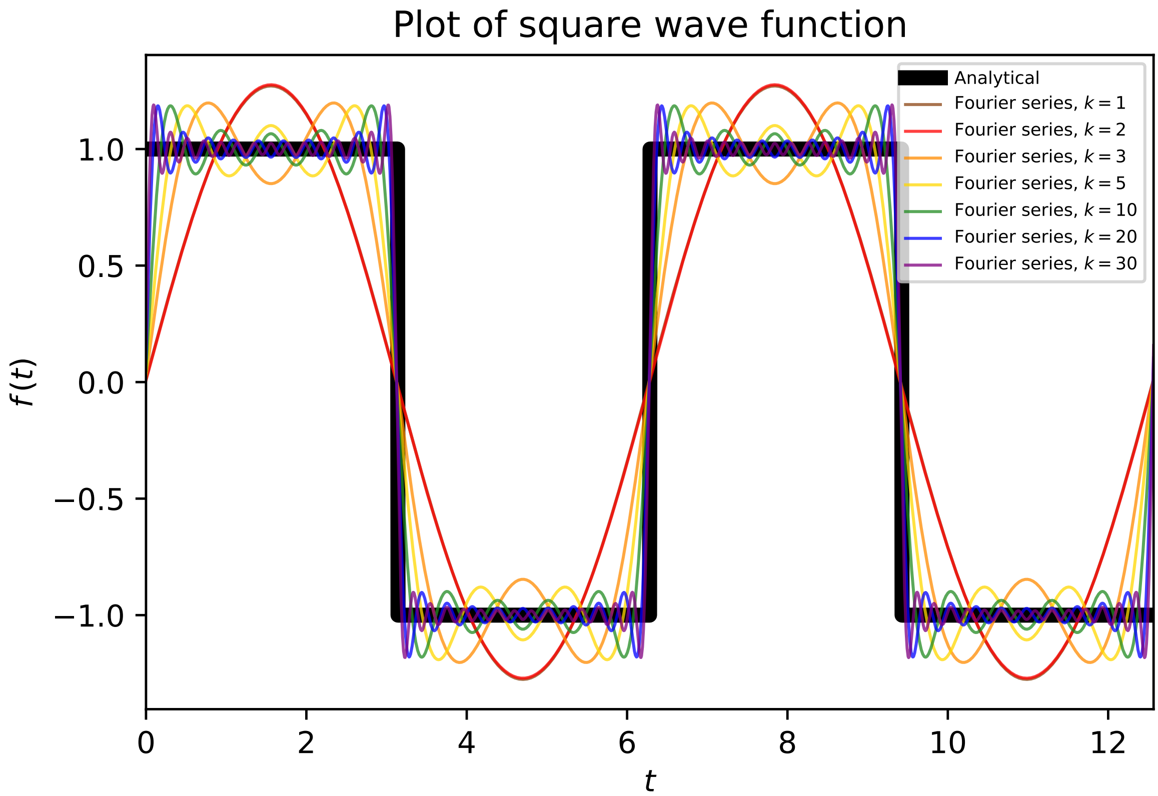
## 3.2 Exercise 2: Fourier Series - Square & Rectangular Wave Functions

The following square and rectangular waves were considered for this exercise:

$$f_{\text{sq}}(t) = \begin{cases} 1, & 0 \leqslant t < \pi \\ -1, & \pi \leqslant t < 2\pi \end{cases} \qquad f_{\text{rec}}(t) = \begin{cases} 1, & 0 \leqslant t < \phi \\ -1, & \phi \leqslant t < 2\pi \end{cases},$$

where $\phi = \frac{1+\sqrt{5}}{2} \approx 1.618$ is the so-called golden ratio.

The following graphs of these functions, and their Fourier series for a variety of numbers of terms, were plotted, with 250 intervals using Simpson's rule:



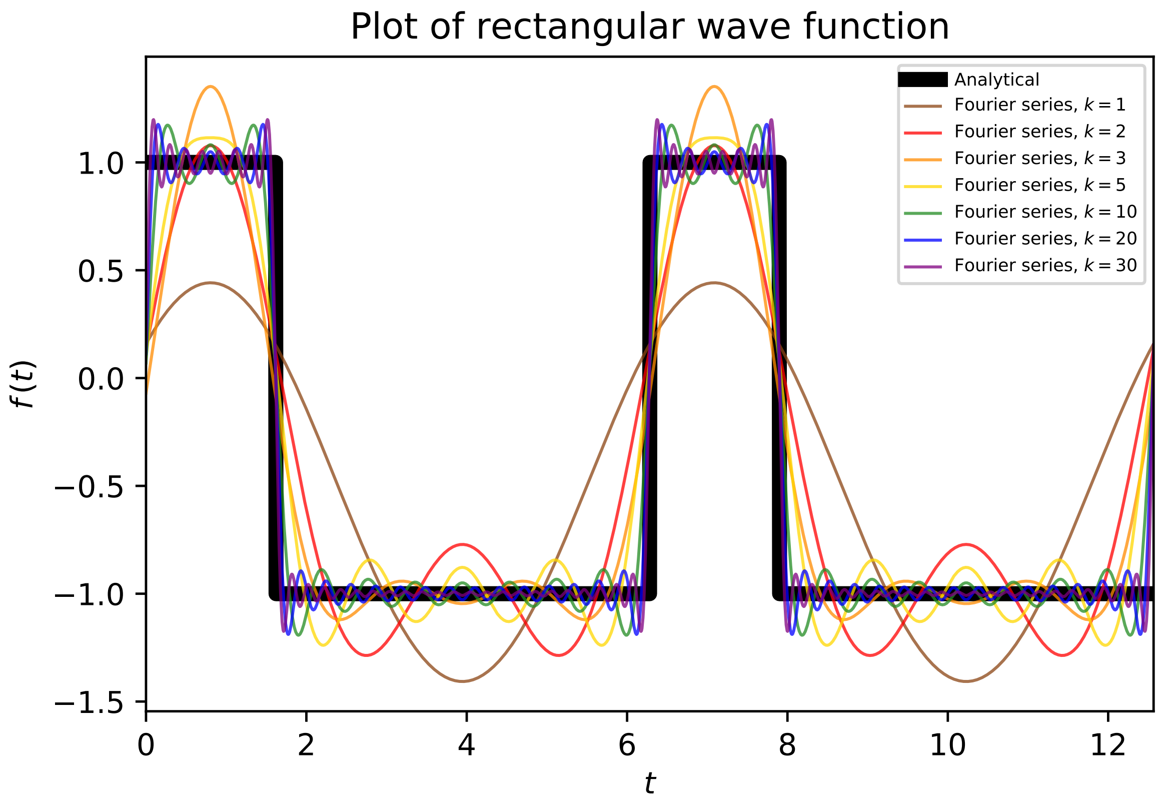




Figure 2: Plot of the square and rectangular wave functions, and their Fourier series, for 1, 2, 3, 5, 10, 20, and 30 terms, using 250 intervals for Simpson's rule.

As can be seen from the graphs in Figure 2, as the number of maximum terms increases, the corresponding Fourier series gets closer to the analytic function. Since the square and rectangular wave functions are not superpositions of sinusoidal functions, they will never be exactly attained after a finite number of terms, but the Fourier series will get nearer with each step.

The following Fourier coefficients were calculated for the square wave function with 5000 intervals for Simpson's rule, and compared to the analytic coefficients using equations (8) - (10):

| $k$ | Analytic $a_k$ | Calculated $a_k$ | Error | Analytic $b_k$ | Calculated $b_k$ | Error |
|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | | | |
| 1 | 0 | 0.0005 | 0.0005 | 1.2732 | 1.2732 | $< 0.0001$ |
| 2 | 0 | $-5 \times 10^{-17}$ | $5 \times 10^{-17}$ | 0 | $-5 \times 10^{-17}$ | $5 \times 10^{-17}$ |
| 3 | 0 | 0.0005 | 0.0005 | 0.4244 | 0.4244 | $< 0.0001$ |
| 4 | 0 | $2 \times 10^{-17}$ | $2 \times 10^{-17}$ | 0 | $-7 \times 10^{-18}$ | $7 \times 10^{-18}$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| 29 | 0 | 0.0005 | 0.0005 | 0.0439 | 0.0439 | $< 0.0001$ |
| 30 | 0 | $-2 \times 10^{-17}$ | $2 \times 10^{-17}$ | 0 | $-8 \times 10^{-18}$ | $8 \times 10^{-18}$ |

Similarly, the following Fourier coefficients were calculated for the rectangular wave function:

| $k$ | Analytic $a_k$ | Calculated $a_k$ | Error | Analytic $b_k$ | Calculated $b_k$ | Error |
|---|---|---|---|---|---|---|
| 0 | $-0.4850$ | $-0.4848$ | 0.0002 | | | |
| 1 | 0.6359 | 0.6362 | 0.0003 | 0.6667 | 0.6667 | $< 0.0001$ |
| 2 | $-0.0300$ | $-0.0298$ | 0.0002 | 0.6352 | 0.6352 | $< 0.0001$ |
| 3 | $-0.2101$ | $-0.2098$ | 0.0003 | 0.1822 | 0.1822 | $< 0.0001$ |
| 4 | 0.0299 | 0.0302 | 0.0003 | 0.0028 | 0.0028 | $< 0.0001$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| 29 | 0.0044 | 0.0046 | 0.0002 | 0.0435 | 0.0435 | $< 0.0001$ |
| 30 | $-0.0210$ | $-0.0207$ | 0.0003 | 0.0245 | 0.0244 | 0.0001 |

As can be seen from these tables, the calculated values of the Fourier coefficients for both wave functions are very close to the analytical values, within a reasonable tolerance. This is due to the fact that a large number of intervals were taken for Simpson's rule; for example, if $n = 250$, as was the case for the graphs in Figure 2, the calculated $a_k$ for the square wave function were as large as 0.016 when they should be 0, and the coefficients for the rectangular wave function had a percentage error of up to 23%.

### 3.3 Exercise 3: Discrete Fourier Transform

The following graphs were obtained for $f_1(t) = \sin(0.45t)$, with $N = 128$ and $h = 0.1$:

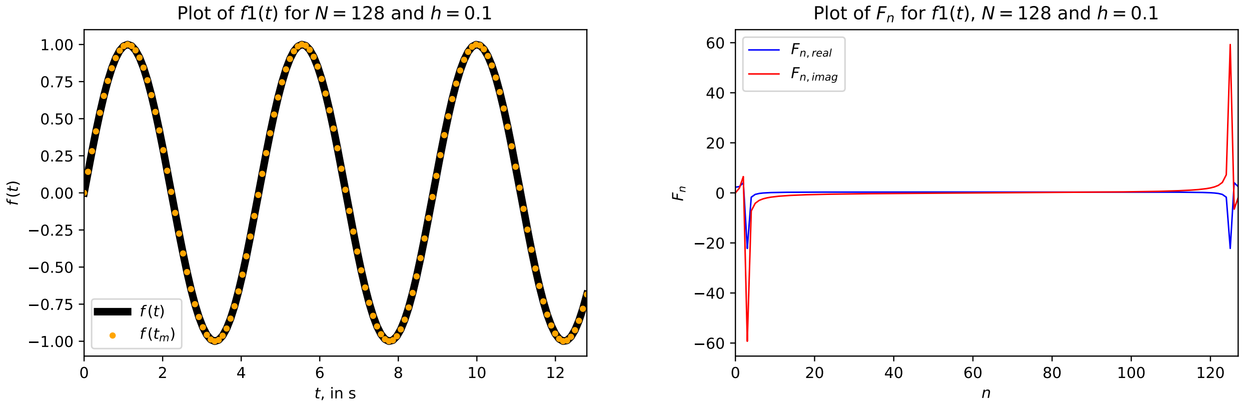



Figure 3: Plot of $f_1(t) = \sin(0.45t)$ with the corresponding sampling points, and the Fourier coefficients $F_n$ in real and imaginary components.

The frequency $\omega$ of $f_1$ is $0.45\pi$, and so an apt choice for $h$ would be $h = \frac{2\pi n}{N\omega} = \frac{5n}{144}$. For this exercise, $h$ was chosen to be $\frac{5}{144} \approx 0.0347$, and $N$ was kept fixed at 128. The following graphs were obtained for $f_1$ and these values of $N$ and $h$:

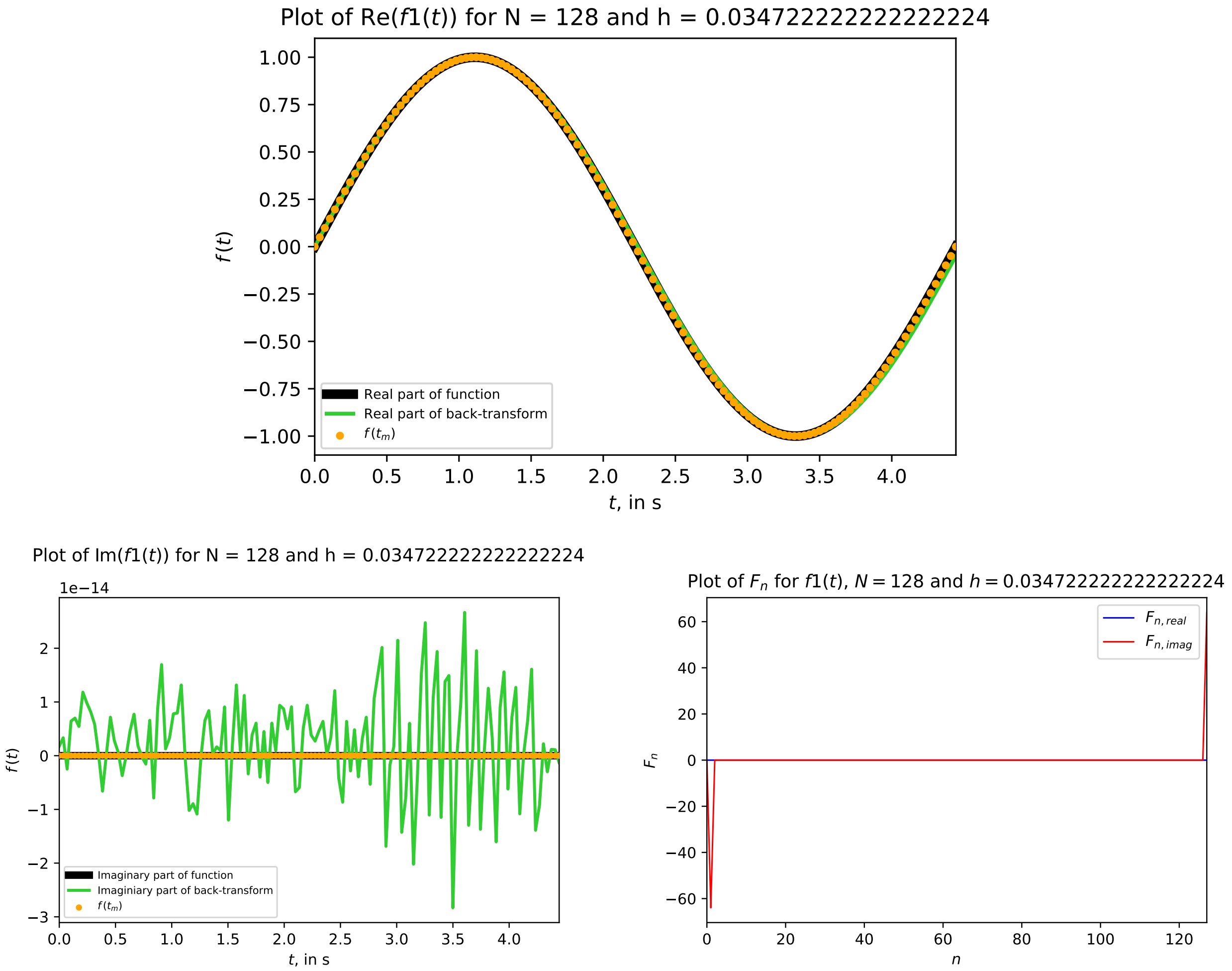



Figure 4: Plot of the real and imaginary part of $f_1(t)$ and the corresponding back-transform, and the Fourier coefficients.

The back-transform of this function almost exactly matches the original function. This is mainly due to the fact that the function itself is periodic, and that both the number of sampling points and the distance between points were optimal choices for this function.

The following graphs were obtained for $f_2(t) = \cos(6\pi t)$ and $N = 32$, with $h = 0.6, 0.2, 0.1, 0.04$:

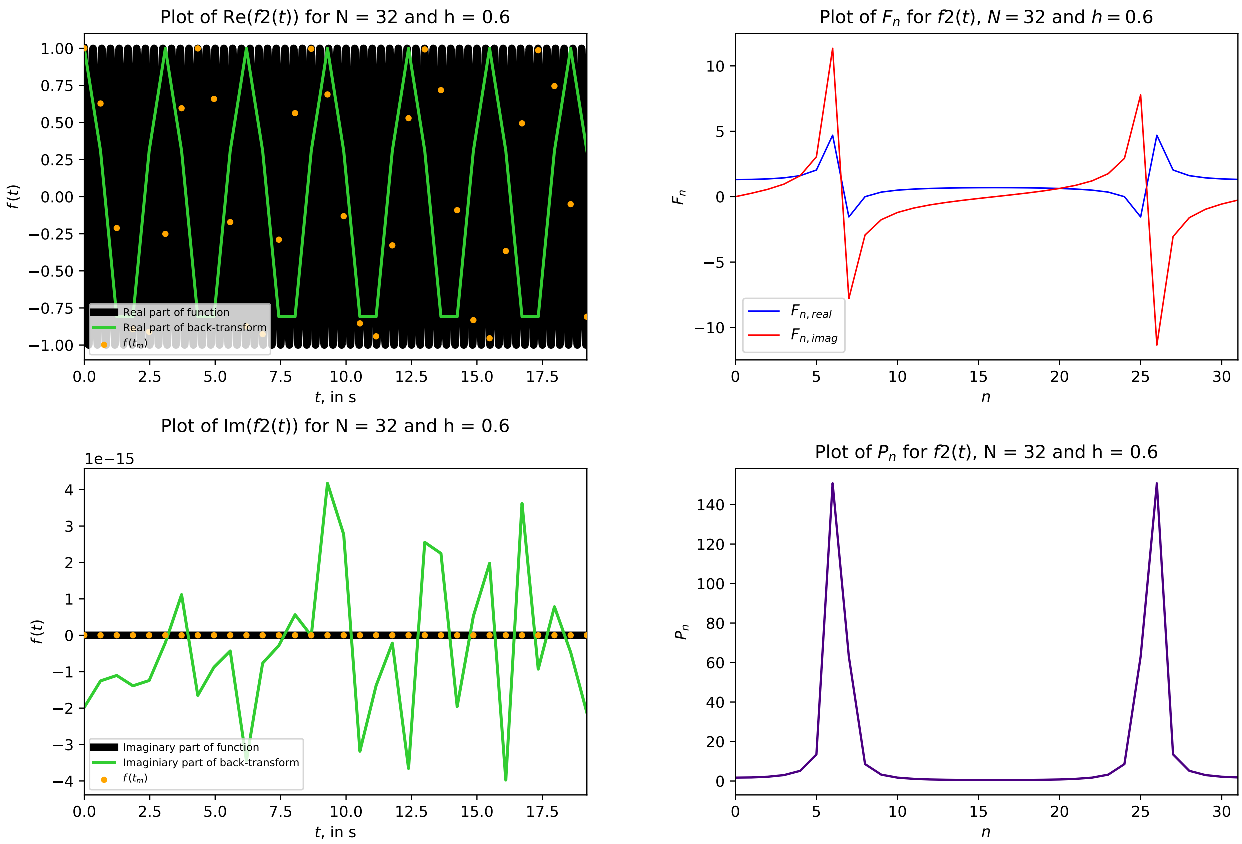



Figure 5: Plot of the real and imaginary components of $f_2(t)$ and its back-transform, the Fourier coefficients, and the power spectrum, for $h = 0.6$.

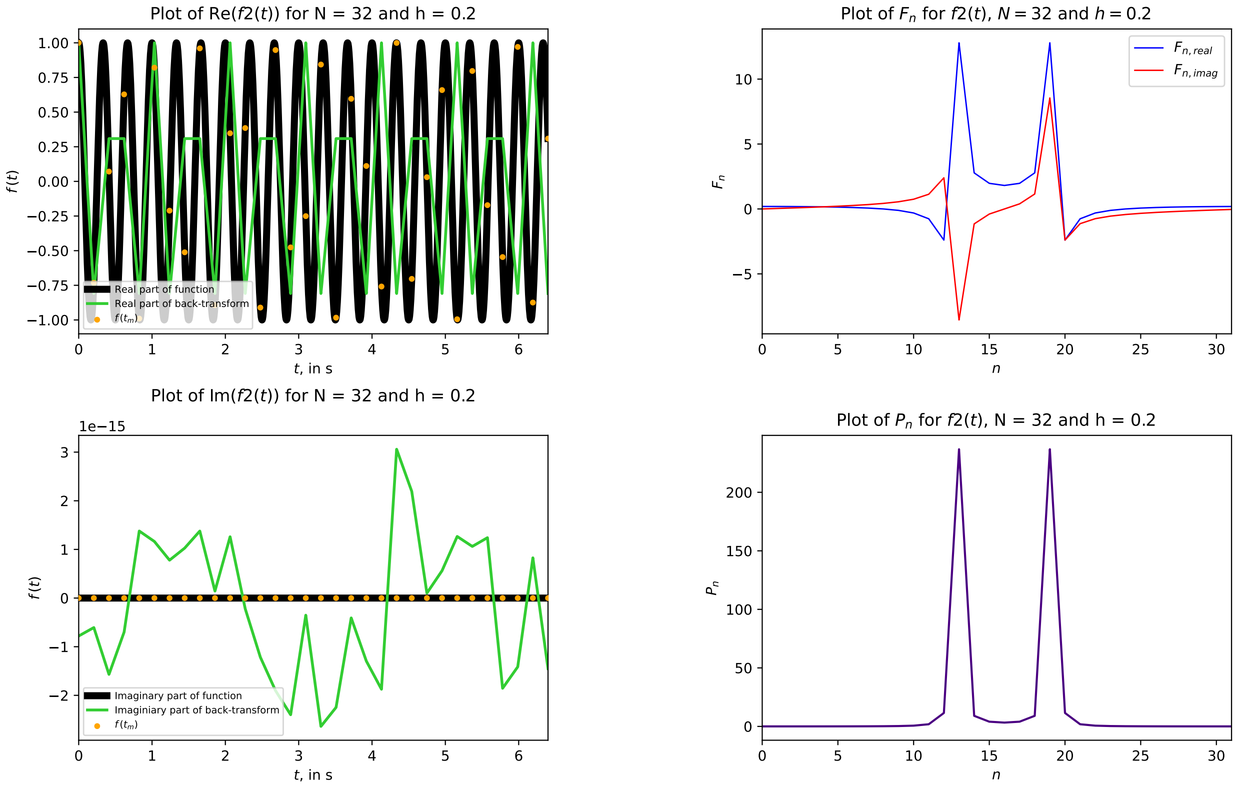



Figure 6: Plot of the real and imaginary components of $f_2(t)$ and its back-transform, the Fourier coefficients, and the power spectrum, for $h = 0.2$.

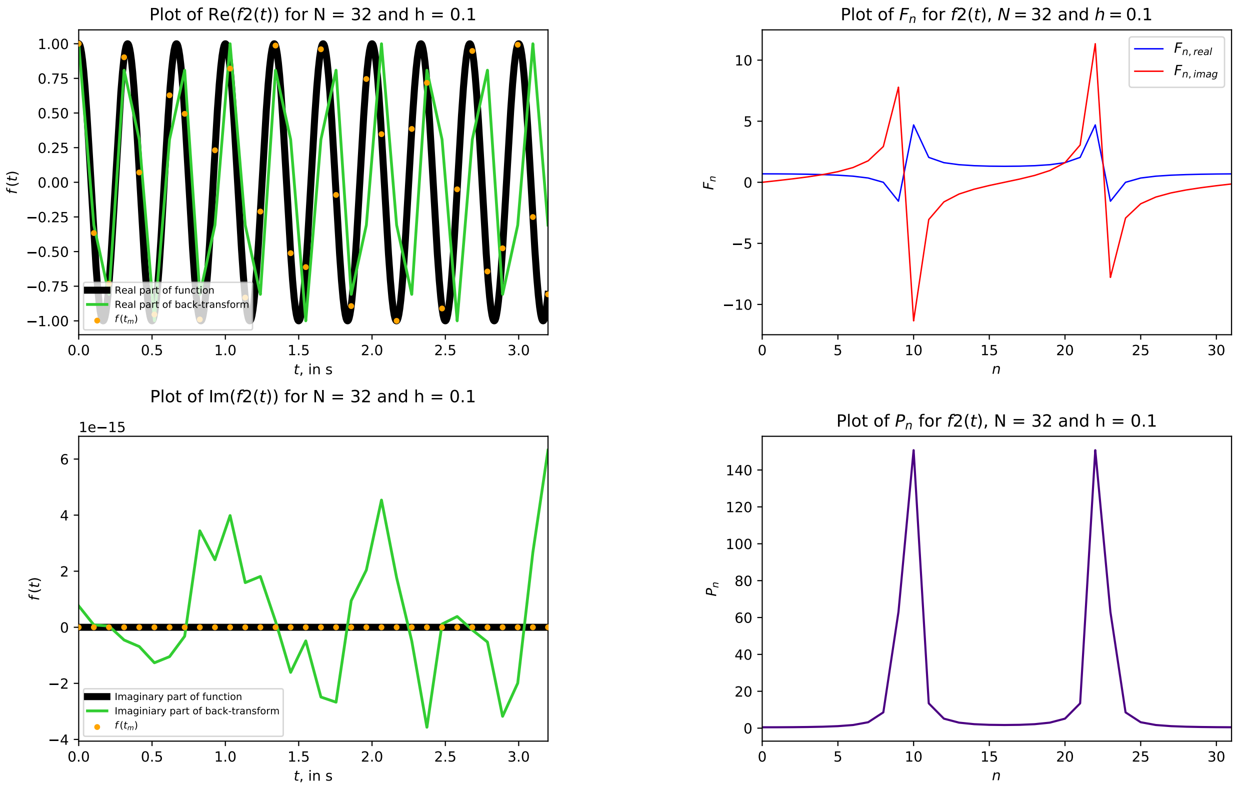



Figure 7: Plot of the real and imaginary components of $f_2(t)$ and its back-transform, the Fourier coefficients, and the power spectrum, for $h = 0.1$.

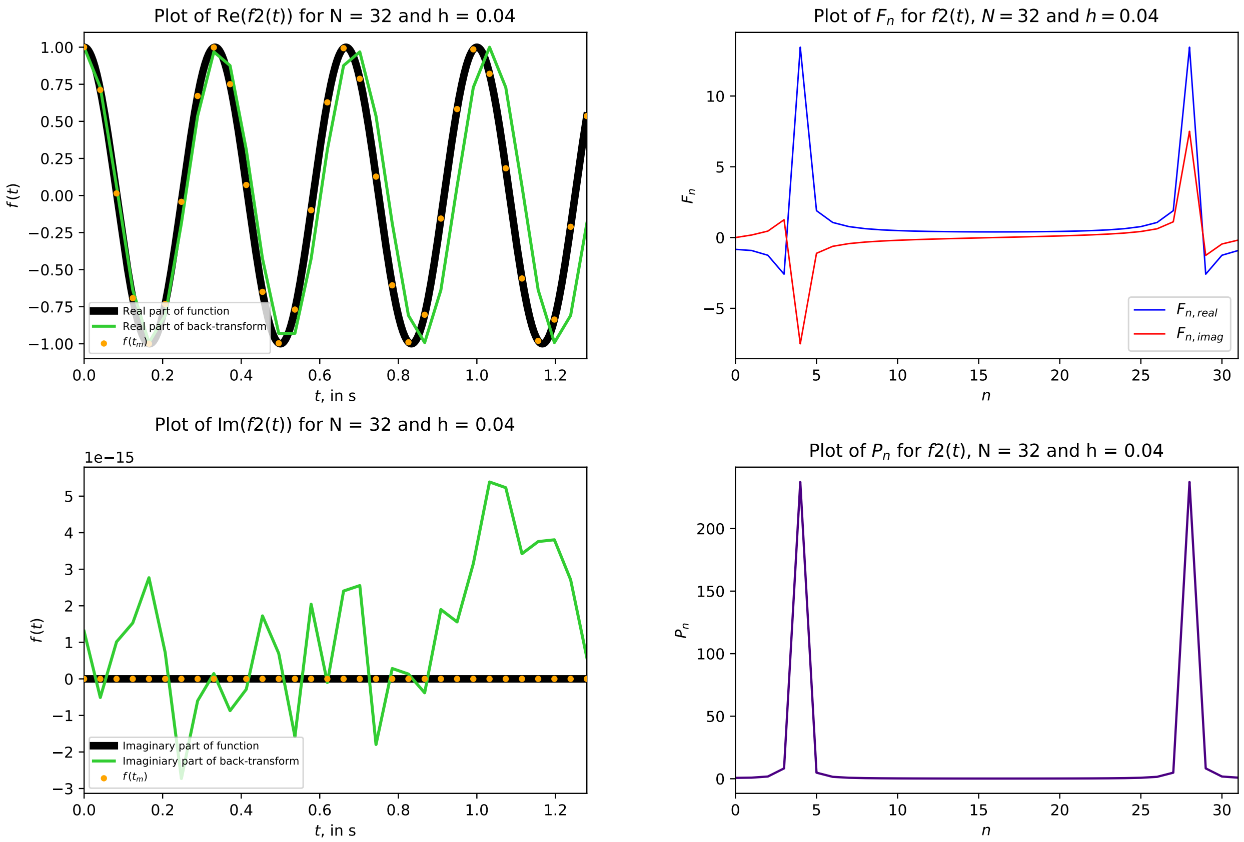



Figure 8: Plot of the real and imaginary components of $f_2(t)$ and its back-transform, the Fourier coefficients, and the power spectrum, for $h = 0.04$.

From Figures 3 - 8, the real and imaginary components of the Fourier coefficients seem to follow a similar pattern, where $\Re(F_n)$ is symmetric about a vertical line, and $\Im(F_n)$ is symmetric about a point. This is due to the so-called Nyquist symmetry, showcased in equation (20), where $F_{N-n} = F_n^*$. The complex conjugate of a complex number has the same real and imaginary magnitudes, but the sign of the imaginary part switches, explaining the patterns in the graphs of $F_n$.

From inspection, the graphs of $F_n$ seem to influence the graphs of the power spectrum. This is as expected, as the power of a signal depends on its frequency, from equation (18). The peaks are due to the corresponding frequency of $f_2(t)$, which is $\omega = 6\pi$. Equating $\omega = \omega_n$ leads to $6\pi = \frac{2\pi n}{Nh}$, or $n = 3Nh$. This explains the location of the peaks in the power spectra and graphs of $F_n$, as $n = 3Nh$ corresponds to $\omega_n = \omega$. Again, there are two peaks in the power spectra due to the conjugate symmetry of $F_n$, as $\Im(F_n)^2 = \Im(F_n^*)^2$.

For $h = 0.6, 0.2$, the corresponding Nyquist frequencies are $\nu = 0.78125, 2.34375$. For each of these values of $h$, the corresponding Nyquist frequency is less than $\frac{\omega}{2\pi} = 3$, and thus the back-transforms of these functions should be less accurate. For $h = 0.1, 0.004$, the Nyquist frequencies are $\nu = 4.6875, 11.71875$. Since these are larger than 3, the corresponding back-transforms should be far more accurate than the previous two. This can be seen in Figures 5 - 8, where the first two back-transforms are very different to the original function, and the last two do a far better job at mimicking the original function.

For each graph of the imaginary part of the back-transform, the amplitude of the function is negligible. This is as expected, as $f_2(t) = \cos(6\pi t)$ has no imaginary parts.

# 4 Conclusions

As was shown in this laboratory, Simpson's rule is an optimal choice of numerical integration method, as the accuracy of the calculations can be chosen from the beginning and altered to one's satisfaction. As with any numerical method, however, a low accuracy corresponds to a large error, and a high accuracy corresponds to a much longer computation time.

For a finite sum of sinusoidal functions it was shown that, although the Fourier series is an infinite sum of sinusoidal functions, it does indeed converge to the original function, with the irrelevant coefficients vanishing to 0. For periodic square and rectangular wave functions, the Fourier series gets closer to the analytic function with each extra pair of terms, and the Fourier coefficients $a_k$ and $b_k$ can be calculated for any $k$.

The discrete Fourier transform can be used in a variety of ways. In this laboratory, it was used to calculate the frequency $\omega$ of a function by inspecting the Fourier coefficients and power spectra. The importance of the Nyquist frequency was also showcased, as when the sampling rate is too small, the Fourier transform has non-negligible inaccuracies, and when the sampling rate is large enough, the transform and back-transform are much better at representing the original function.

# 5 References & Appendix


1: J. Fourier, *Mémoire sur la propagation de la chaleur dans les corps solides*, Nouveau Bulletin des Sciences par la Société philomathique de Paris, pp. 215 - 221, December 1807.

2: TCD School of Physics, provided laboratory instructions, April 2021.

3: Wolfram MathWorld, `https://mathworld.wolfram.com/NyquistFrequency.html`, accessed April 2021.


All code and figures used in this laboratory can be found here:
`https://github.com/campioru/SF_Lab_4`