Lab 1: Monte Carlo Methods

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1 Introduction

2 Methods

Fourier series are defined by calculating the fourier coefficients a_n and b_n. These coefficients may be replaced when in a complex Fourier series using a term c_n. Using the following equations:

$$\begin{aligned} a_n =& c_n + c_{-n} \\ b_n =& i(c_n - c_{-n}) \\ c_n =& \frac{1}{2}(a_n - ib_n) \end{aligned} \tag{1}$$

In fourier series, the a_n and b_n correspond to even and odd 'components' of the function. In the case of an even function:

$$\begin{aligned} a_n =& c_n + c_{-n} \\ b_n =& 0 \\ c_n =& \frac{1}{2}(a_n) \end{aligned} \tag{2}$$

And for odd functions:

$$\begin{aligned} a_n =& 0 \\ b_n =& i(c_n - c_{-n}) \\ c_n =& \frac{-ib_n}{2} \end{aligned} \tag{3}$$

It may be shown in both of the above series that the a_n term for even functions and b_n for odd functions will be proportional to the c_n terms.

Next, a square wave function was considered as defined below:

$$f(t) = \begin{cases} 1, & |t| \le T/4 \\ 0, & |t| > T/4 \end{cases}$$

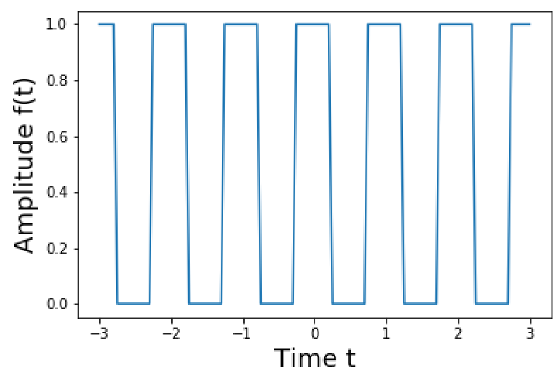

Figure 1: A square wave function. The period of the function has been set to $T = 1$, periodic from $T = -1/2$ to $T = 1/2$.

This function was periodic between $-T/2$ and $T/2$. The function was visualized in figure 1. As with any function, this could be re-stated using complex Fourier series. To compute the series, the coefficients c_n were determined according to equation 4.

$$c_n = \frac{1}{T}\int_{-T/2}^{T/2} f(t)\exp(-i\frac{2\pi nt}{T})dt \tag{4}$$

The coefficients could be solved analytically, yielding the answer $c_n = \frac{-i}{\pi n}$ for $n = 1, 3, 5, \ldots.$ As the found n values suggest, the original function was purely odd, meaning that the function could be constructed from purely sine terms. Due to this, all even c_n terms (including c_0) are 0. The values of the different c_n terms may also be plotted, as shown in figure 2. The values in this plot show that the odd n terms follow a hyperbolic sinusoid path. The complete se-

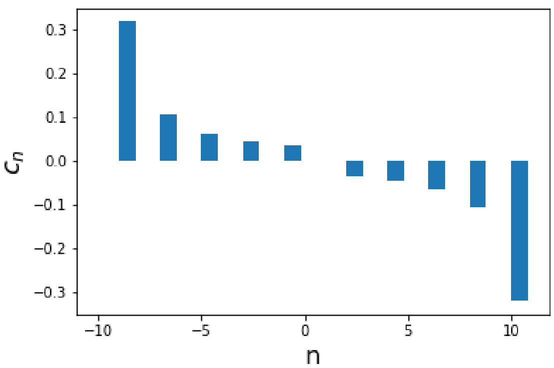

Figure 2: Values of each term c_n in the complex fourier series.

ries may be written as:

$$f(t) = \sum_{n=-\infty}^{\infty} -\frac{i}{\pi n} \exp(-i\frac{2\pi nt}{T})$$

2.1 Noise

2.1.1 Autocorrelation and PSD

The autocorrelation function was examined in a previous lab. It turns out that the auto-correlation function may be applied to random signals (i.e. noise) as well. For white noise created from a uniform distribution of frequencies, the autocorrelation function is expected to be a delta function. Consider an ideal random number generator separate from the realities of computing. By definition, a number correlates with itself completely, forming a spike at $k = 0$. For ideal noise, there is no relation between the first number generated, and any subsequent number generated. This means that subsequent values should yield $k = 0$. Taken together, this is a description of $\delta(k)$.

The power spectral density function is connected to the auto-correlation function by the following formula:

$$S(\omega) = \sum_{-\infty}^{\infty} AC(k)e^{-j\omega k}$$

Using this, the PSD of white noise may be calculated:

$$S(\omega) = \sum_{i=-\infty}^{\infty} \delta(k)e^{-j\omega k} S(\omega) = \delta(k=0)e^{-j\omega * 0} S(\omega) = 1$$

The above mathematical relations were tested

2.2 Spectral Subtraction

The spectral subtraction method involved Fourier transforming a signal, and then setting frequency bin values to zero if they were below a certain threshold. A signal was created using the formula $x(t) = \sin(2\pi f_0 t) + 0.5\sin(2\pi(2f_0)t)$ using $f_0 = 440$ Hz sampled at $22.2\mu s$, for 512 intervals. Figure3a shows this signal. The power spectrum of the signal was found using numpy's FFT package. Figure 3b shows this corresponding power spectrum. Two clear peaks were visible at 0.00976 and 0.01953. This matches almost exactly the expected values of 0.9768 and 0.19536 obtained by multiplying the frequency by the sampling period.

To investigate the impact of noise on the signal, random noise on the order ± 0.5 was added to the signal. Figures 3c and 3d show the noisy power spectrum. The noise in this power spectrum was almost imperceptible compared to the signal in the neighborhood of the expected peaks. By outputting the power data, it was seen that the noise was on the order of 10^{-1}. Some noise was slightly beyond one order of magnitude above or below this, indicating that the noise was not 'ideal' white noise.

Next, the threshold at which the magnitude of the noise cause the underlying signal to be totally obscured was determined. This was done by steadily increasing the noise magnitude until the signal peaks were on the order of the peaks from noise. Figure 3e and 3f show the corresponding signal and power spectrum.

2.2.1 Signals with Trends

In this section, a periodic signal was laid over a linear trend to produce a new function. The original periodic function was $x_i = 2\sin(\pi f_0 i) + \cos(\pi f_1 i)$ while the trend function was $g(i) = 1 + 0.025i$ (constants of $f_0 = 9/512$ and $f_1 = 4/512$ were used). When added together, the two functions produced a new function, visualized in figure 4. Next, the signal was made noisy using uniform noise of ± 6 added to the function. Figure **??** shows the result.

As earlier in this lab, the FFT was used to examine the data for the underlying periodicity. Figure 6 showed the resulting power spectrum. The data was confined to a single, massive spike at $f = 0$. For a noisy signal, the noise would be expected to manifest as a uniform addition across the power spectrum. This would still allow the original frequencies to be recovered. The lack of any distinct periodic peaks (the $f = 0$ peak corresponds to non-periodic components) suggests that the linear component has erased the ability to check periodicity in the power spectrum.

While it has been shown that the periodicity of the data are obscured, it might have still been possible to remove the noise across all frequencies, and attempt to recover the original, noiseless function. To attempt this, all frequencies with a magnitude of less than 180 were removed. Figure 7 shows the result. Clearly this method has not been successful.

Next, a different method of uncovering the original $x(i)$ function was attempted. First, the $g(i)$ term was removed from $x(i)$. This new modified $x(i)$ was then Fourier transformed. The noise was again removed from the signal using only frequency magnitudes greater that 180. It was found that using the suggested filtering value of 9 from the lab instructions did not yield the correct results. Using the filtered frequency spectrum, the inverse Fourier transform, that is the noiseless $x(i) - g(i)$ was obtained. Finally, the trend $g(i)$ was added back to the signal. Originally, this yielded a massive sinusoid without upward trend. To fix this, after the frequency spectrum was returned to the time domain, the result was renormalized to the maximum of the original trend-less $x(i)$. This was cheating somewhat, as in real experiments, the maximum of the original function might not be known. Once the signal was re-normalized and had $g(i)$ added back in, the signal behaved more similarly to what was expected. Figure **??** shows the final result.

2.2.2 Autocorrelation and Power Spectra

The autocorrelation function and the power spectrum of signals are related. This may be demonstrated analytically with relative ease. Essential to these derivations is the Fourier shift theorem. The theorem provides a quick way to simply a Fourier transform when the function in question contains a shift in the coordinate being transformed. The theorem is derived below:

$$\begin{aligned}\mathcal{F}\{f(t-a)\} &= \int_{-\infty}^{\infty} f(t-a)e^{2\pi i\omega t}dt \\ &= \int_{-\infty}^{\infty} f(t-a)e^{2\pi i\omega t}e^{2\pi i\omega a}e^{-2\pi i\omega a}dt \\ &= e^{2\pi i\omega a}\int_{-\infty}^{\infty} f(t-a)e^{2\pi i\omega t}e^{-2\pi i\omega a}dt \\ &= e^{2\pi i\omega a}\int_{-\infty}^{\infty} f(t-a)e^{2\pi i\omega (t-a)}dt \\ &= e^{2\pi i\omega a}\int_{-\infty}^{\infty} f(t')e^{2\pi i\omega t'}dt' \\ &= e^{2\pi i\omega a}\mathcal{F}\{f(t)\}\end{aligned} \tag{5}$$

First, a proof will be shown for $C(\omega) = \sqrt{2\pi}Y^*(\omega)X^*(\omega)$:

$$
\begin{aligned}
c(\tau) =& \int_{-\infty}^{\infty} y^*(t-\tau)x(t)dt \\
\mathcal{F}\{c(\tau)\} =& \mathcal{F}\{\int_{-\infty}^{\infty} y^*(t-\tau)x(t)dt\} \\
C(\omega) =& \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} y^*(t-\tau)x(t)e^{2\pi i\omega\tau}dtd\tau \\
=& \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} y^*(-\tau)x(t)e^{2\pi i\omega t}e^{2\pi i\omega\tau}dtd\tau \\
=& \int_{-\infty}^{\infty} y^*(\tau)e^{2\pi i\omega(-\tau)}d\tau \int_{-\infty}^{\infty} x(t)e^{2\pi i\omega t}dt \\
=& \sqrt{2\pi}Y^*(\omega)X(\omega)
\end{aligned} \tag{6}
$$

Related to the correlation function is the autocorrelation function. The autocorrelation function may be defined as a convolution of a function with itself. From this term's Fourier material, it has been stated that a convolution in one space is a product in the corresponding Fourier space. From this, the relation between the autocorrelation and the power spectrum of a signal have been linked. This may be proved, as shown below:

$$
\begin{aligned}
AC(\tau) =& \int_{-\infty}^{\infty} y^*(t)y(t+\tau)dt \\
\mathcal{F}\{AC(\tau)\} =& \mathcal{F}\{\int_{-\infty}^{\infty} y^*(t-\tau)y(t)dt\} \\
AC(\omega) =& \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} y^*(t-\tau)y(t)e^{2\pi i\omega\tau}dtd\tau \\
=& \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} y^*(-\tau)y(t)e^{2\pi i\omega t}e^{2\pi i\omega\tau}dtd\tau \\
=& \int_{-\infty}^{\infty} y^*(\tau)e^{2\pi i\omega(-\tau)}d\tau \int_{-\infty}^{\infty} y(t)e^{2\pi i\omega t}dt \\
=& \sqrt{2\pi}Y^*(\omega)Y(\omega) \\
=& \sqrt{2\pi}|Y(\omega)|^2
\end{aligned} \tag{7}
$$

The auto-correlation function of white noise was explored earlier in this assignment. The findings of that computation may be verified analytically. Given that white noise should exist equally at all, infinite frequencies in the frequency domain, the autocorrelation may be determined by reverse Fourier transform. To begin, an assumption is made that the power of all frequencies is $S(f) = k$.

$$
\begin{aligned}
S(f) =& k \\
AC(\tau) =& \mathcal{F}^{-1}\{S(f)\} \\
AC(\tau) =& \sqrt{2\pi}\int_{-\infty}^{\infty} ke^{-2\pi i f\tau}df \\
AC(\tau) =& \sqrt{2\pi}k\int_{-\infty}^{\infty} e^{-i\omega\tau}\frac{d\omega}{2\pi} \\
AC(\tau) =& \frac{k}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-i\omega\tau}d\omega \\
AC(\tau) =& \frac{k}{\sqrt{2\pi}}\delta(\tau)
\end{aligned} \tag{8}
$$

2.3 Applications

2.3.1 The Lorenz System

The Lorenz system is a description of physical systems where a large number of variables are interrelated through differential equations. For this example, a system with three variables and three parameters will be considered. Equations 9 shows the system of equations in question.

$$
\begin{aligned}
\frac{\partial x}{\partial t} =& \sigma(y-x) \\
\frac{\partial y}{\partial t} =& rx - y - xz \\
\frac{\partial y}{\partial t} =& xy - bz
\end{aligned} \tag{9}
$$

The equation will reach an equilibrium in the case where all the partial derivatives are zero. The x, y, and z equilibrium values may be found analytically:

$$
\begin{aligned}
0 = \sigma(y-x) \quad &\rightarrow \quad x = y \\
0 = xy - bz \quad &\rightarrow \quad y = \sqrt{(bz)} \\
0 = rx - y - xz \quad &\rightarrow \quad z = r - 1 \\
\therefore x = y =& \sqrt{(b(r-1))}
\end{aligned} \tag{10}
$$

2.3.2 ODEs and the Fourier Transform

The Fourier transform can be use to reduce the dimensionality of a differential equation. In essence, if the fourier transform is used, a PDE with two different differentials may be reduced to an ODE or and ODE to a polynomial equation. The original solution may then be recovered by reverse transforming the result. Below are a few examples of simplifying differential equations through Fourier transform:

$$\begin{aligned} &\mathcal{F}\{m\ddot{x} + D\dot{x} + \kappa x = n(t)\} \\ &-\omega^2\hat{x} + i\omega\hat{x} + \kappa\hat{x} = \hat{n}(\omega) \end{aligned} \tag{11}$$

$$\begin{aligned} &\mathcal{F}\{ih\frac{\partial\psi}{\partial t} + \frac{h^2}{2m}\frac{\partial^2\psi}{\partial x^2} = 0\} \\ &-\omega h\hat{\psi} - \frac{ih^2}{2m}\frac{\partial^2\hat{\psi}}{\partial x^2} = 0 \end{aligned} \tag{12}$$

$$\begin{aligned} &\mathcal{F}\{\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial z^2} = \delta(x)\delta(z-a)\} \\ &-k^2\hat{T} + \frac{\partial^2\hat{T}}{\partial z^2} = e^{-2\pi ikx}\delta(z-a) \end{aligned} \tag{13}$$

2.3.3 Heat Equation

A common differential equation that is difficult to solve with non-complex analysis was the heat equation. The heat equation was defined as:

$$\begin{aligned} \frac{\partial^2 T}{\partial x^2} &= -q(x) \\ q(x) &= \frac{\exp(-(x-x_0)^2/(2\sigma^2))}{\sqrt{2\pi\sigma^2}} \end{aligned} \tag{14}$$

This equation may be re-written using Fourier analysis. Two aids were used in this analysis: an integral table result for a zero-mean gaussian transform [4], and the Fourier shift theorem to take care of the x_0 shift. Equations 15 show this process.

$$\begin{aligned} &\mathcal{F}\{\frac{\partial^2 T}{\partial x^2}\} = \mathcal{F}\{-q(x)\} \\ &-k^2\hat{T} = -\hat{q}(x) \end{aligned}$$

$$\begin{aligned} \hat{q}(x) &= \mathcal{F}\{\frac{\exp(-(x-x_0)^2/(2\sigma^2))}{\sqrt{2\pi\sigma^2}}\} \\ \hat{q}(x) &= e^{-2\pi ikx_0} \times \mathcal{F}\{\frac{\exp(-(x^2/(2\sigma^2))}{\sqrt{2\pi\sigma^2}}\} \\ \hat{q}(x) &= \exp\left(\frac{-\sigma^2k^2}{2} - 2\pi ikx_0\right) \\ \hat{T} &= \frac{1}{k^2}\exp\left(\frac{-\sigma^2k^2}{2} - 2\pi ikx_0\right) \end{aligned} \tag{15}$$

In order to obtain a solution to the heat equation, a reverse transform could be applied on the above equation to return the original heat function.

3 Conclusion

References

[1] Ouyed and Dobler, PHYS 581 course notes, Department of Physics and Astrophysics, University of Calgary (2016).

[2] W. Press et al., *Numerical Recipes* (Cambridge University Press, 2010) 2nd. Ed.

[3] C. Hass and J. Burniston, MCMC Hill Climbing. Jupyter notebook, 2018.

[4] K. Derpanis, Fourier Transform of the Gaussian, 2005, accessed at `http://www.cse.yorku.ca/~kosta/CompVis_Notes/fourier_transform_Gaussian.pdf`.

4 Appendix

For access to the source codes used in this project, please visit `https://github.com/Tsintsuntsini/PHYS_581` for a list of files and times of most recent update.

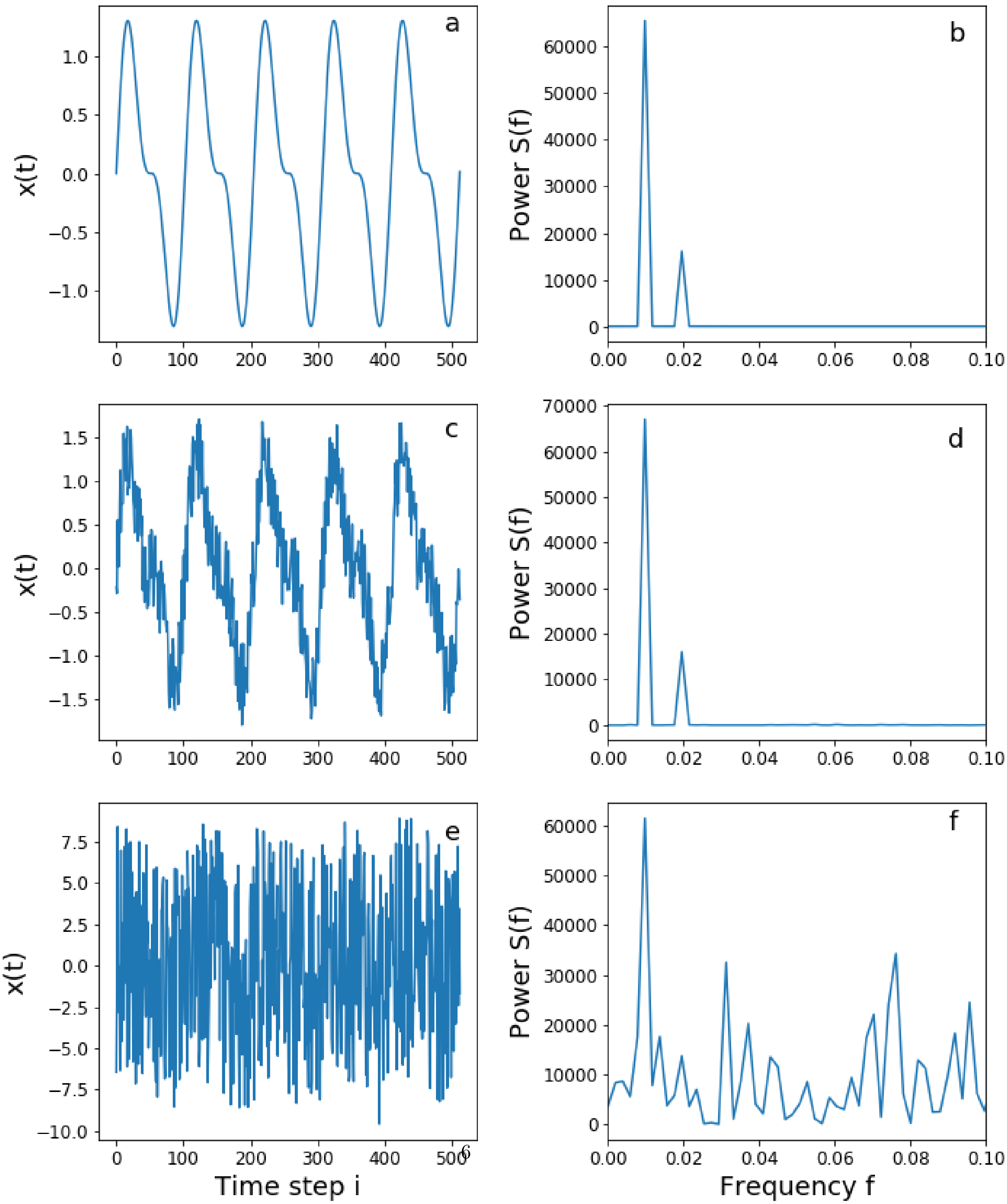

Figure 3: Effects of uniformly distributed (in time space) noise on a signal. Subplot **a** shows the original input signal, subplot **c** a signal with noise of ± 0.5 from the original signal, and subplot **e** the signal with ± 10 noise. The subplots immediately to the right are the corresponding frequency power spectra.

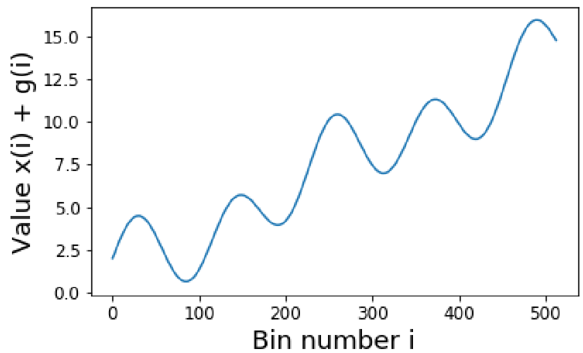

Figure 4: Function obtained by adding together a periodic and a linear function.

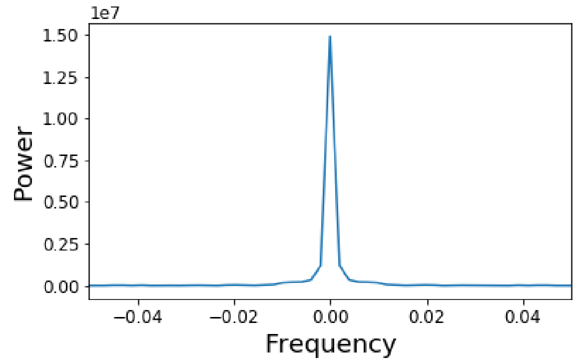

Figure 6: FFT of the noisy function in figure 5. The result was focused on the region near $f = 0$ to ensure that there were not peaks close to $f = 0$. Regions outside this window continued at an amplitude of approximately zero. Note that the amplitude axis is scaled by a factor of 10^7.

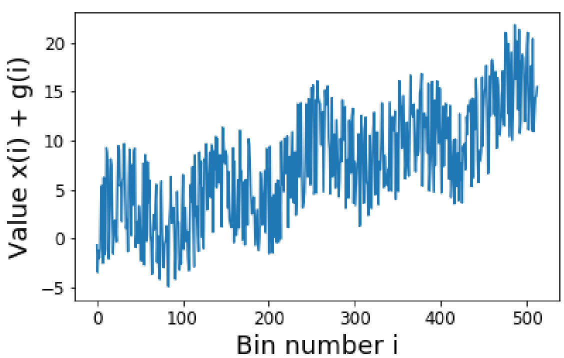

Figure 5: Function from figure 4 with uniform noise applied.

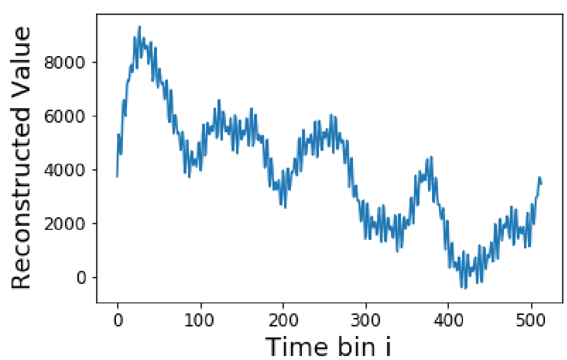

Figure 7: Reconstruction of the signal in figure 4 using an inverse FFT. Note that the trend $g(i)$ does not appear as expected in the reconstruction. This result was one of many: each separate run of the program produced a different reconstruction based on the different random noise changes.

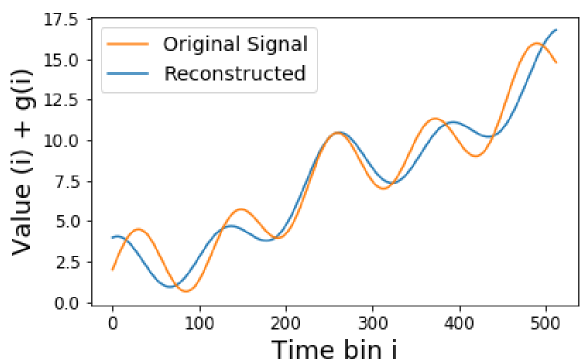

Figure 8: Reconstruction of the original signal from figure 4. Note the aparent scale difference between the two lines.