Lab 1: Monte Carlo Methods

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1 Introduction

The Fourier transform is one of the mathematical marvels of the modern world. While it was invented in the early 19th century, it was instrumental in the communication's revolution beginning with radio, and continuing into the modern digital world. The Fourier transform is an extension of the fourier series, which expresses a function in terms of a basis of sinusoids or exponentials. The Fourier transform allows one to work on a problem either in its original space or in that of a Fourier space. There are many pairs of variables that may be connected by Fourier transform including time/frequency and position/wavenumber. By working in Fourier space, certain periodic patterns may be emphasized or de-emphasized in data. This is the basis of modern signal processing and filtering to remove noise. Fourier techniques have myriad applications outside the mathematical context of this assignment including audio-processing, radio-astronomy, and medical imaging.

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:

$$a_{n} = c_{n} + c_{-n}$$

 $b_{n} = i(c_{n} - c_{-n})$
 $c_{n} = \frac{1}{2}(a_{n} - ib_{n})$
(1)

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

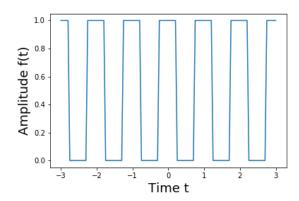


Figure 1: A square wave function. The period of the function has been set to T=1, periodic from T=-1/2 to T=1/2.

an even function:

$$a_n = c_n + c_{-n}$$

$$b_n = 0$$

$$c_n = \frac{1}{2}(a_n)$$
(2)

And for odd functions:

$$a_n = 0$$

$$b_n = i(c_n - c_{-n})$$

$$c_n = \frac{-ib_n}{2}$$
(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.

Parseval's theorem relates the Fourier coefficients of a function to its power spectrum. Using the above relations, it may be restated in terms of sine and cosine coefficients, as shown below.

$$\int_{-\infty}^{\infty} |x(t)|^2 dt = \sum_{n=-\infty}^{\infty} |c_n|^2$$

$$\sum_{-\infty}^{\infty} |c_n|^2 = \sum_{n=-\infty}^{\infty} |\frac{1}{2} (a_n - ib_n)|^2$$

$$= \frac{1}{2^2} \sum_{n=-\infty}^{\infty} (a_n - ib_n) (a_n + ib_n)$$

$$= \frac{1}{2^2} \sum_{n=-\infty}^{\infty} |a_n|^2 + |b_n|^2$$

$$= \frac{1}{2^2} \sum_{n=0}^{\infty} |a_n|^2 + |b_n|^2$$

$$= \frac{|a_0|^2}{2^2} + \frac{1}{2^2} \sum_{n=1}^{\infty} |a_n|^2 + |b_n|^2$$

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

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

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 5.

$$c_n = \frac{1}{T} \int_{-T/2}^{T/2} f(t) \exp(-i\frac{2\pi nt}{T}) dt$$
 (5)

The coefficients could be solved analytically, yielding the answer $c_n = \frac{-i}{\pi n}$ for n=1,3,5,... 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 series may be written as:

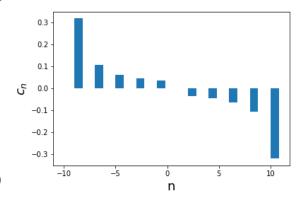


Figure 2: Values of each term c_n in the complex fourier series.

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

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:

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

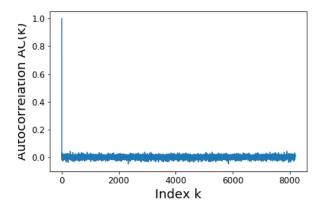


Figure 3: Autocorrelation function from uniform numbers generated using numpy's random.rand() function.

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 using uniform random numbers on the interval [0,1). For 8192 numbers, the auto-correlation and associated power spectral density were plotted in figures 3 and 4. In order for these plots to behave as expected, the algorithm for auto-correlation provided in lab 1 required modification. The original algorithm for each k summed over terms $1 \to N - k$. This meant that higher k values were subject to wide fluctuations due to deceasing denominator terms. By writing the algorithm to consider all other random numbers except the 'kth' random number in sums, the results were as expected. The power spectral density fluxuated, but had a mean of 0.969 near the expected $S(\omega) = 1$.

Calculation of the auto-correlation function and PSD was repeated for white noise generated by a Gaussian distribution. Figures 5 and 6 show the results obtained. The PSD had a mean value of 1.07.

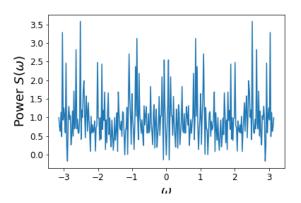


Figure 4: Power spectrum density of white noise created from uniform random numbers. The auto-correlation values in figure 3 were used to calculate the PSD.

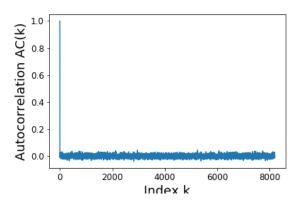


Figure 5: Autocorrelation function of white noise generated by random Gaussian numbers.

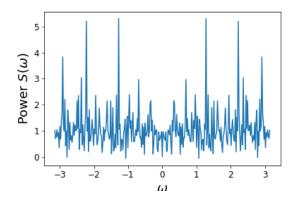


Figure 6: Power spectral density of random white noise generated from a Gaussian distribution. This plot was created using autocorrelation data from figure 5.

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. Figure 7a shows this signal. The power spectrum of the signal was found using numpy's FFT package. Figure 7b 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 7c and 7d 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 ob-

scured 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 7e and 7f 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 8. 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 10 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 11 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:

$$\mathcal{F}\{f(t-a)\} = \int_{-\infty}^{\infty} f(t-a)e^{2\pi i\omega t}dt$$

$$= \int_{-\infty}^{\infty} f(t-a)e^{2\pi i\omega t}e^{2\pi i\omega a}e^{-2\pi i\omega a}dt$$

$$= e^{2\pi i\omega a} \int_{-\infty}^{\infty} f(t-a)e^{2\pi i\omega t}e^{-2\pi i\omega a}dt$$

$$= e^{2\pi i\omega a} \int_{-\infty}^{\infty} f(t-a)e^{2\pi i\omega(t-a)}dt$$

$$= e^{2\pi i\omega a} \int_{-\infty}^{\infty} f(t')e^{2\pi i\omega t'}dt'$$

$$= e^{2\pi i\omega a} \mathcal{F}\{f(t)\}$$
(6)

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

$$c(\tau) = \int_{-\infty}^{\infty} y^*(t - \tau)x(t)dt$$

$$\mathcal{F}\{c(\tau)\} = \mathcal{F}\{\int_{-\infty}^{\infty} y^*(t - \tau)x(t)dt\}$$

$$C(\omega) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} y^*(t - \tau)x(t)e^{2\pi i\omega\tau}dtd\tau$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} y^*(-\tau)x(t)e^{2\pi i\omega t}e^{2\pi i\omega\tau}dtd\tau$$

$$= \int_{-\infty}^{\infty} y^*(\tau)e^{2\pi i\omega(-\tau)}d\tau \int_{-\infty}^{\infty} x(t)e^{2\pi i\omega t}dt$$

$$= \sqrt{2\pi}Y^*(\omega)X(\omega)$$
(7)

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:

$$AC(\tau) = \int_{-\infty}^{\infty} y^*(t)y(t+\tau)dt$$

$$\mathcal{F}\{AC(\tau)\} = \mathcal{F}\{\int_{-\infty}^{\infty} y^*(t-\tau)y(t)dt\}$$

$$AC(\omega) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} y^*(t-\tau)y(t)e^{2\pi i\omega\tau}dtd\tau$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} y^*(-\tau)y(t)e^{2\pi i\omega t}e^{2\pi i\omega\tau}dtd\tau$$

$$= \int_{-\infty}^{\infty} y^*(\tau)e^{2\pi i\omega(-\tau)}d\tau \int_{-\infty}^{\infty} y(t)e^{2\pi i\omega t}dt$$

$$= \sqrt{2\pi}Y^*(\omega)Y(\omega)$$

$$= \sqrt{2\pi}|Y(\omega)|^2$$
(8)

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.

$$S(f) = k$$

$$AC(\tau) = \mathcal{F}^{-1} \{ S(f) \}$$

$$AC(\tau) = \sqrt{2\pi} \int_{-\infty}^{\infty} k e^{-2\pi i f \tau} df$$

$$AC(\tau) = \sqrt{2\pi} k \int_{-\infty}^{\infty} e^{-i\omega \tau} \frac{d\omega}{2\pi}$$

$$AC(\tau) = \frac{k}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega \tau} d\omega$$

$$AC(\tau) = \frac{k}{\sqrt{2\pi}} \delta(\tau)$$

$$(9)$$

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 10 shows the system of equations in question.

$$\frac{\partial x}{\partial t} = \sigma(y - x)$$

$$\frac{\partial y}{\partial t} = rx - y - xz$$

$$\frac{\partial y}{\partial t} = xy - bz$$
(10)

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:

$$0 = \sigma(y - x) \rightarrow x = y$$

$$0 = xy - bz \rightarrow y = \sqrt{(bz)}$$

$$0 = rx - y - xz \rightarrow z = r - 1$$

$$\therefore x = y = \sqrt{(b(r - 1))}$$
(11)

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:

$$\mathcal{F}\{m\ddot{x} + D\dot{x} + \kappa x = n(t)\}\$$

$$-\omega^{2}\hat{x} + i\omega\hat{x} + \kappa\hat{x} = \hat{n}(\omega)$$
(12)

$$\mathcal{F}\{ih\frac{\partial\psi}{\partial t} + \frac{h^2}{2m}\frac{\partial^2\psi}{\partial x^2} = 0\}$$
$$-\omega h\hat{\psi} - \frac{ih^2}{2m}\frac{\partial^2\hat{\psi}}{\partial x^2} = 0$$
 (13)

$$\mathcal{F}\left\{\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial z^2} = \delta(x)\delta(z-a)\right\}$$

$$-k^2 \hat{T} + \frac{\partial^2 \hat{T}}{\partial z^2} = e^{-2\pi i k x}\delta(z-a)$$
(14)

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:

$$\frac{\partial^2 T}{\partial x^2} = -q(x)$$

$$q(x) = \frac{\exp(-(x - x_0)^2 / (2\sigma^2))}{\sqrt{2\pi\sigma^2}}$$
(15)

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 16 show this process.

$$\mathcal{F}\left\{\frac{\partial^2 T}{\partial x^2}\right\} = \mathcal{F}\left\{-q(x)\right\}$$

$$-k^2 \hat{T} = -\hat{q}(x)$$
(16)

In order to numerically solve the heat equation, the function q(x) should be Fourier transformed to obtain $\hat{q}(k)$. This term may then be divided by k^2 and reverse transformed to obtain the original T(x). This yields a problem in the case where k=0. Since python interprets a division by zero by returning 'nan', replacing this 'nan' with some DC term will allow the inverse transform to perform correctly. Figure 13 shows the result of performing this method. Since the 'DC' term for k=0 has been replaced, this is not the exact answer, and instead is shifted by the non-existent DC term. It was therefore possible to shift this data so that all points had a nonnegative temperature by shifting by the global minimum value.

The limits of Fourier transform solutions were considered using the function q(x) = 0. For this case, the familiar solution of T(x) = Ax + B was obtained using analytical methods. For this particular case, the Fourier method of solutions breaks down. If we were to Fourier transform q(x), the result would be q(k) = 0. This in turn would lead to an overall solution T(x) = 0. This is a valid solution for the analysis above in the case A = B = 0, however it is only one possible solution out of many. One way to consider this special case is that in its transformed form the Fourier inverse of temperature is \hat{q}/k^2 . This acts to have a delta-esqe peak at zero frequency, except in the case where $\hat{q} = 0$. To consider this from another direction, the fourier transform of the analytical solution was $\mathcal{F} = B\sqrt{(2\pi)}\delta(k) - iA\sqrt{(2\pi)}\delta(k)$ so the only information in Fourier space was contained at k=0, where the special case of q=0 removes the peaks.

3 Discussion

Different representations of the Fourier series can orovide different ways of looking at the same problem. While cosines and sines are useful for the initiate, the most common representation is the exponential representation. Section 2 above showed the connection between complex and sinusoidal coefficients. These relationships are related to the 'even' and 'uneven' aspects of a function in question. The a coefficient

represents the even part of a function, while the b coefficients describe odd parts. This means that the c coefficients are directly related to the a and b coefficients for even and odd functions, respectively. This can allow for a better intuition of results. An example of this was provided by a piecewise odd function. Since the function was odd, all of the a terms vanished as may be seen in figure 2, where the b terms survived.

Sampling windows and noise work to change a continuous source into the imperfect signal that many experiments rely upon. Where noise is extremely difficult to remove in the time domain, the frequency domain allows characterization of noise. In this experiment, the power spectra of different types of white noise were examined. White noise was characterized in the Frequency domain by an relatively uniform distribution of frequencies in theory. In actuality, the power spectra exhibited quite a bit of fluctuation around the expected mean of $S(\omega) = 1$. This was likely due to three factors. First, the numpy random number generator used is known to be a poor random number generator. Secondly, all purely computational random number generators are actually pseudo-random, and will not exactly obey expectations. Lastly, the noise sample taken was somewhat limited in duration. As the noise sample length increases, the auto-correlation value will more closely approach zero beyond k = 0 since for most numbers the denominator will grow faster than the numerator in the AC equation.

Another method for examining noise was spectral subtraction. By transforming a signal into the frequency domain, the periodic signals will have well defined peaks compared to noise, which will allow data below a threshold to be removed, and the original signal to be recovered, with some error. This error is due to the impact of noise on a particular peak being difficult to evaluate. The experiments above showed that a signal must be significantly smaller than the amplitude of noise before it is well hidden. The above experiment found that the signal was still visible in the frequency domain until the noise was an order of magnitude larger than the signal. This is a relief for many in physics, as this means spectral isolation of signals can occur for even faint signals.

Trends were seen to be an effective way to mask the spectral signature of a signal. The peak caused by a trend tended to completely obscure underlying frequency data, and rendered spectral subtraction largely useless. If the equation of the trend is known, subtracting the trend from the original signal allowed underlying frequency data to be seen with some error. This suggests a rather simple method for encrypting data, which may be decrypted by a recipient with knowledge of the trend. An interesting test for a future experiment would be to test the effectiveness of least squares methods in effectively determining a trend.

The Fourier transform was shown to be a technique to transform many differential equations into algebraic equations. Many simple differential equations were turned into quadratic equations which would be quickly solvable in one's head. While simple differential equations are made quite trivial with this method, they were already solvable with calculus methods. Where Fourier transforms really shine however, is with non-homogeneous differential equations. Non-homogeneous differential equations often required complicated methods to solve, and many were not solvable. If a function modifying a homogeneous equation was Fourier transformable, it had the possibility of being solved in the frequency domain, where the equation might be easier.

A transformed differential equation, specifically the heat equation, was examined. In this case, the boundary values made analytical solving of the transformation integral difficult. This was overcome by numerically evaluating a Gaussian function q(x) on the interval $0 \le x \le 1$ and then using a fast Fourier transform to evaluate it. In the frequency domain, the \hat{T} function could then be obtained by dividing by k^2 . This however demonstrated a difficulty in using Fourier analysis to solve differential equations. When dividing by some variable, one must ensure that variable is not zero. Hence, an analytical solution was not possible for this differential equation, since it was possible for k to equal zero. This is somewhat navigible however, as the k=0 term only yields a constant shift in the x domain. As long as the system has some initial condition for T, the missing vertical shift should be recoverable.

4 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.

5 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.

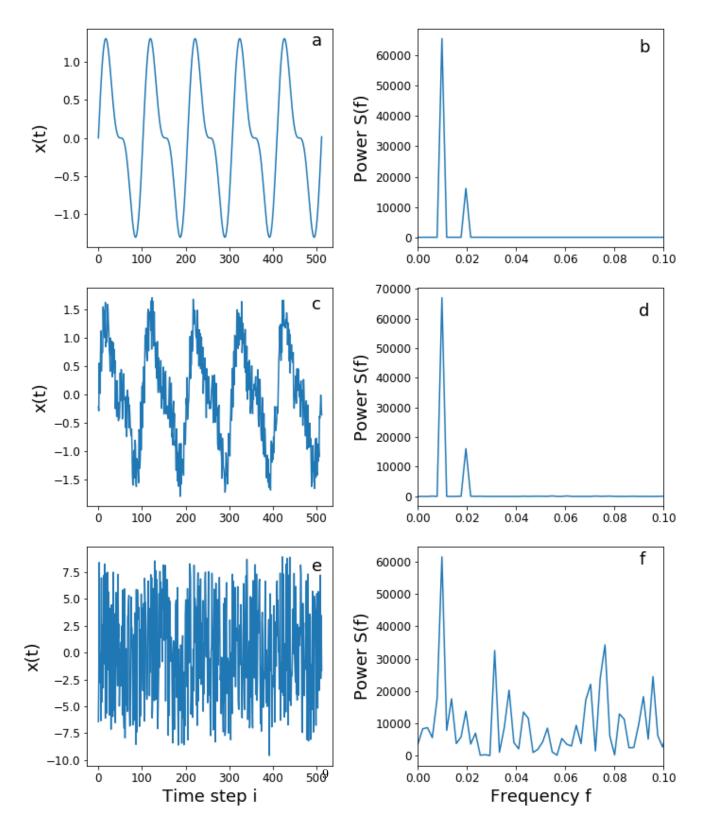


Figure 7: Effects of uniformly distributed (in time space) noise on a signal. Subplot $\bf a$ shows the original input signal, subplot $\bf c$ a signal with noise of ± 0.5 from the original signal, and subplot $\bf e$ the signal with ± 10 noise. The subplots immediately to the right are the corresponding frequency power spectra.

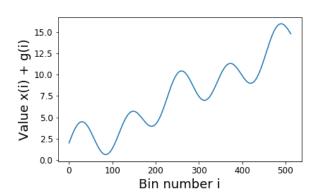


Figure 8: Function obtained by adding together a periodic and a linear function.

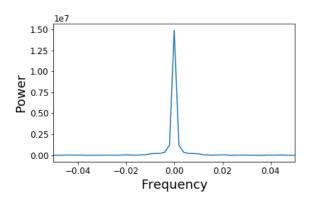


Figure 10: FFT of the noisy function in figure 9. The result was focused on the region near f=0 to ensure that there were not peaks close to f=0. Regions outside this window continued at an amplitude of approximately zero. Note that the amplitude axis is scaled by a factor of 10^7 .

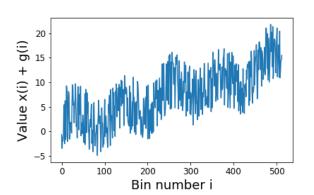


Figure 9: Function from figure 8 with uniform noise applied.

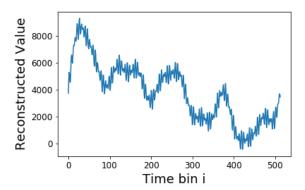


Figure 11: Reconstruction of the signal in figure 8 using an inverse FFT. Note that the trend g(i) does not appear as expected in the reconstruction. This result was one of many: each separate run of the program produced a different reconstruction based on the different random noise changes.

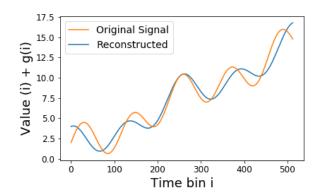


Figure 12: Reconstruction of the original signal from figure 8. Note the aparent scale difference between the two lines.

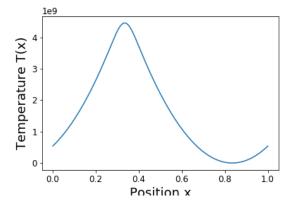


Figure 13: Temperature of a length 1 rod corresponding to equation ??. The temperature may be off by a constant shift due to the deletion of the DC component in the frequency space.