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:

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

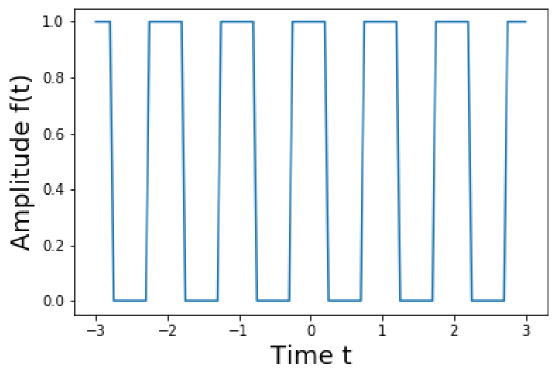

Figure 1: A square wave function. The period of the function has been set to $T = 1$, periodic from $T = -1/2$ to $T = 1/2$.

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 $n = 1, 3, 5, ...$. 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-

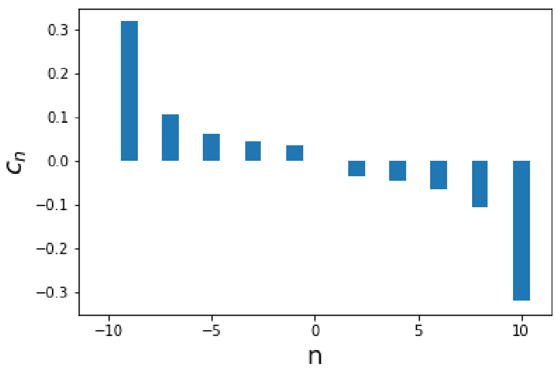

Figure 2: Values of each term c_n in the complex fourier series.

ries may be written as:

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

2.1 Applications

2.1.1 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:

$$\begin{aligned} &\mathcal{F}\{m\ddot{x} + D\dot{x} + \kappa x = n(t)\} \\ &-\omega^2\hat{x} + i\omega\hat{x} + \kappa\hat{x} = \hat{n}(\omega) \end{aligned} \tag{5}$$

$$\begin{aligned} &\mathcal{F}\{ih\frac{\partial\psi}{\partial t} + \frac{h^2}{2m}\frac{\partial^2\psi}{\partial x^2} = 0\} \\ &-\omega h\hat{\psi} - \frac{ih^2}{2m}\frac{\partial^2\hat{\psi}}{\partial x^2} = 0 \end{aligned} \tag{6}$$

$$\begin{aligned} &\mathcal{F}\{\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial z^2} = \delta(x)\delta(z-a)\} \\ &-k^2\hat{T} + \frac{\partial^2\hat{T}}{\partial z^2} = e^{-2\pi i k x}\delta(z-a) \end{aligned} \tag{7}$$

2.1.2 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:

$$\begin{aligned} \frac{\partial^2 T}{\partial x^2} &= -q(x) \\ q(x) &= \frac{\exp(-(x-x_0)^2/(2\sigma^2))}{\sqrt{2\pi\sigma^2}} \end{aligned} \tag{8}$$

This equation may be re-written using Fourier analysis:

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

$$\begin{aligned} \hat{q}(x) =& \mathcal{F}\{\frac{\exp(-(x-x_0)^2/(2\sigma^2))}{\sqrt{2\pi\sigma^2}}\} \\ \hat{q}(x) =& e^{-2\pi i k x_0} \times \mathcal{F}\{\frac{\exp(-(x^2/(2\sigma^2))}{\sqrt{2\pi\sigma^2}}\} \\ \hat{q}(x) =& \exp\left(\frac{-\sigma^2 k^2}{2} - 2\pi i k x_0\right) \\ \hat{T} =& \frac{1}{k^2}\exp\left(\frac{-\sigma^2 k^2}{2} - 2\pi i k x_0\right) \end{aligned} \tag{9}$$

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 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.