Developing a Better Procedure for Lattice Data Analysis

A thesis submitted in partial fulfillment of the requirement
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by

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Abstract

Quantum chromodynamics is a type of Quantum Field Theory that describes the strong nuclear force and the interactions of particles such as protons and neutrons. Systems in QCD are strongly coupled, and therefore, we cannot have exact results and need to use numerical computation of path integrals. In QCD, we are frequently interested in extracting particle masses from correlation functions. But the computer-generated data have large errors, and following upon this, when we fit the data with our expected model, the large uncertainties get carried over to the parameters. In this way the obtained quantities are sometimes not that useful to be compared with experimental results. We see if fitting the same data with wavelets can improve their precision. Wavelets improve the uncertainties of the constant term in the parameters, but I have doubt on whether it is the same thing as the asymptote of the data, the quantity of our interest.

Chapter 1

Introduction

1.1 The Goal of the Project

Quantum Field Theory (QFT) is a theoretical formulation that combines quantum mechanics and special relativity. We want to solve systems in QFT, and for some of the systems, we rely on numerical techniques. QFT describes any theory that is built from quantum fields. Quantum Chromodynamics (QCD) is one type of QFT that describes the strong nuclear force, the force that operates in the interaction between protons and neutrons. At low energies, QCD is strongly coupled, which means that we cannot use perturbation theory, an approximation method, to leave off other not very probable interactions and concentrate on the dominating one. Short of a direct analytical solution to the system or an approximating one, we numerically calculate the relations within the system. This numerical calculation just means statistics: when we have a large enough sample size, we can see how a system would act by looking at its typical, or average, behavior.

By applying this technique, we can compute quantities in the system inside the proton. Since theory is to be compared to experiments to test the theory, we want to calculate what can be compared with experimental results. In experiments, the main way to study the internal structure of protons and neutrons is deep inelastic scattering (DIS). The process of DIS is that an electron or muon is shot off at high velocity past a proton, and on its way it sends a photon towards the proton, which causes it to break up into new particles, while the electron scatters off from the interaction. One of the quantities that can be probed through DIS experiments is parton distribution functions (PDFs). A PDF is the probability of finding a certain fraction of momentum carried by a specific quark, or all of the gluons, inside the proton. The function takes a specified fraction of the proton momentum as its input.

But to theoretically calculate PDFs brings up a difficulty. The data for PDFs have large uncertainties, and thus when we want to fit the data with an equation of PDFs, the resulting fitting parameters have large uncertainties. A good range of values could pass within the predicted range of the quantity, which makes its comparison with experimental results unproductive.

The study of this report is on how we can make more precise predictions of the value of quantities like PDFs. Specifically, we study if fitting the computational data under the wavelet basis would be better than with the theoretical equation of how the data should go, which, in our case, is an exponential function of time multiplied once by time itself. We use two wavelet bases, one discrete and one continuous, and show how well they apply to the data. We will also compare it with the fit under the Fourier basis.

I want to explain the reason we set out testing the wavelet basis. We believe wavelets can help us reduce the uncertainties in the parameters because wavelets provide adjustable ranges for fitting. I will provide more details on wavelets in the theory section and give the expressions for the two wavelet bases we used in our tests. In zeroing in on the time-frequency components of a function, wavelets give clearer results than Fourier series. Therefore, we believe they can capture the important information of a function better, that is, can reconstruct it closer to its original shape.

The organization of this report is as follows: first, in the theory section, I give a little more description of QFT, the context in which our research is situated. I talk about what wavelets are and their difference from Fourier series. Then, I show our results of fitting results using the analytical expression, Fourier basis, and wavelets respectively, where we are interested in extracting the value of PDFs. Finally, I am going to discuss and conclude from our results whether wavelets are a promising tool for people interested in the same goal.

Chapter 2

Theory

2.1 Quantum Field Theory (QFT)

Quantum Field Theory (QFT) describes any theory that is built from quantum fields. QFT holds two principles: it says that, first, quantum fields are operator-valued functions that transform in specific ways under the Lorentz group, and, second, that the interactions of the fields are local. It is a break-away from Newtonian mechanics where fields are generated by other objects. In QFT, one can describe the behavior of an object without referring to distant other objects.

QFT brings a number of things to the preexisting theories. It 1) uniquely explains the existence of different, yet indistinguishable, copies of elementary particles, 2) gives each class of those indistinguishable particles a unique quantum statistics, 3) tells us of the existence of anti-particles, 4) explains the local interactions as the products of operators at a point, and 5) explains the forces exerted by the classical fields as the result of exchange of particles [1].

2.2 The Path Integral

The path integral is equivalent to the Schrödinger equation for non-relativistic quantum mechanics. It can tell us all the information about a quantum system. For example, one quantity is the propagator. If we start a wave-function $\psi(x)$ at the position x_i in the position eigenstate $|x_i\rangle$, let it evolve in time, the probability that it will be at x_f after time t can be calculated by the path integral

$$P(x_i, x_f, t) = \langle x_f|e^{-\hat{H}t}|x_i\rangle. \tag{2.1}$$

$P(x_i, x_f, t)$ is the propagator. This is after we change to Euclidean space from Minkowski space so that $it \to t$.

People have proved that this can be written as the integration of all the paths that lead from x_i to x_f weighted by the factor $e^{-S[x]}$. Here, S is the action:

$$S[x] = \int_{t_i}^{t_f} dt[\frac{m\dot{x}}{2} + V(x(t))]. \tag{2.2}$$

We would describe a path by selecting some points and drawing lines between them. If we have N points in every path, i.e., turning each path x into $x = \{x_1, x_2, ..., x_N\}$, the path integral becomes

$$P(x_i, x_f, t) = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 ... \int_{-\infty}^{\infty} dx_{N-1} e^{-S[x_1]} ... e^{-S[x_{N-1}]}. \tag{2.3}$$

The action is discretized onto the points $x_1, x_2, ..., x_N$. We stop at $N-1$ because we are thinking of a situation where $x_f = x_i$, i.e., the endpoints are fixed. The numerical equation 2.3 will be equal to the exact expression 2.1 when $N \to \infty$.

The path integral is the approach to generate Lattice QCD data, and the data I am analyzing comes from Lattice QCD. I studied generating data from the path integral in a one-dimensional system in the first semester.

2.3 Wavelets

2.3.1 General Description

A wavelet basis is usually called a family. This clever analogy tells us their important characteristics: they resemble each other but are of different sizes, like Russian dolls. In more scientific language, the other terms in the basis come from translating and/or compressing or expanding a mother wavelet $\psi(x)$. They are in the form of $\psi(\frac{x-b}{a})$, where b translates the mother wavelet and a scales it.[2]

The wavelet transform is like the Fourier transform. The Fourier transform converts an input into an infinite series of sines and cosines and gives us their coefficients. The wavelet transform does the same thing; it expresses the function in the wavelet basis, in the form of a superposition of the terms of that basis.

The purpose of the Fourier transform is to get the frequency components and how much they each contribute to the function, which is their coefficients. But there are times when we also want to know a third thing: when these frequencies appear, like telling a musician when to play the note besides telling them what note it is and at how much volume. The way to do it in Fourier transform is by viewing the function through a window, cropping out the rest of the time scale and data. Then when we do Fourier transform, we get the frequency components of the function in that time interval, which is a small segment of time, almost making the result representative of every instant within it. The expression for this procedure is:

$$T^{win}_{m,n} = \int dx\ f(x)\ g(x - nx_0)\ e^{-im\omega_0 x} \tag{2.4}$$

where $T^{win}_{m,n}$ is a shorthand meaning windowed Fourier transform, $f(x)$ is the function we are looking at, x_0 is the step size when we slide the window by steps, for the frequency components within the window at each location, n is the number of steps we have moved the window by – this is the discrete, i.e., implementable, version; in the continuous one, we would imagine the window smoothly scans across $f(x)$. Here m is the number of steps when we replace ω with $\omega = m\omega_0$, from the expression for the standard Fourier transform:

$$\tilde{f}(\omega) = \int dx\, e^{-i\omega x}\, f(x). \tag{2.5}$$

[2] Now, in Eq.2.4, $g(s-t_0)\, e^{-im\omega_0 s}$ is the window we look out from at the function. It is an envelope $g(s-t_0)$ filled up by $e^{-im\omega_0 s}$. As we change the mode m, the folds become dense or more spaced apart, but the envelope size does not change, which means every Fourier basis function covers the same range of $f(s)$.

In contrast, wavelet basis functions are compressed or dilated from the mother wavelet, and the terms where a is large are narrow, and where a is small are broad. When there is a quick change in the function, the narrow term will be a big component; and when the function is smooth like the wave of the sea, the broad term in the basis will carry more weight. It is this variation of scale that makes a wavelet basis different from the Fourier basis and better at fitting to certain functions.

2.3.2 Haar and Morlet Wavelets

The two wavelet bases we have used in our fitting attempts are Haar and Morlet Wavelets [2][3]. Haar Wavelet is a group of functions scaled and translated from a square wave:

$$\psi(x) = \begin{cases} 1 & 0 \le x \le \frac{1}{2} \\ -1 & \frac{1}{2} \le x \le 1 \\ 0 & x \text{ equals other values} \end{cases} \tag{2.6}$$

Then when we scale it by powers of 2 and translate it, the resulting general expression is

$$\psi_{j,k}(x) = 2^{-j/2}\, \psi(2^{-j}x - k) \tag{2.7}$$

where j is related to the index of the power, and k is the how much the function gets moved transversely. j and k are integers, but we can choose their values.

This is a case of a discrete function. We have also used a continuous one – the Morlet Wavelets, given below,

$$\psi(x) = c_\sigma \, \pi^{-1/4} \, e^{-\frac{1}{2}t^2} \, (e^{i\sigma t} - \kappa_\sigma). \tag{2.8}$$

[3] In this equation, the constants c_σ and κ_σ are related to σ by

$$c_\sigma = (1 + e^{-\sigma^2} - 2\, e^{-\frac{3}{4}\sigma^2})^{-\frac{1}{2}} \tag{2.9}$$

and

$$\kappa_\sigma = e^{-\frac{1}{2}\sigma^2}. \tag{2.10}$$

In my case right now, I am using $\sigma = 2$. Either the real or the imaginary part of Morlet wavelets is a sinusoidal wave whose peaks are traced out by a Gaussian curve, as we can see from the two components of t within the function Eq. 2.8. I took the sine wave or the imaginary part of this equation to build my basis, though I am sure the real part, the cosine wave, would not make a difference.

To increase $\psi(t)$ into a family, it is translated and/or scaled:

$$\psi_{a,b}(x) = |a|^{-\frac{1}{2}} \, \psi(\frac{t-b}{a}), \tag{2.11}$$

where a and b are given by

$$a = 2^m, \tag{2.12}$$

$$b = n\, 2^m, \tag{2.13}$$

with m, n ranging over Z (integers) [2].

I have put in plots of a Haar mother wavelet in Fig. 2.1 and a Morlet wavelet in Fig. 2.2 that I downloaded off of wikipedia.

Here I have presented the expressions of wavelets, which I then coded into the fit function through a superposition of some of them from a basis.

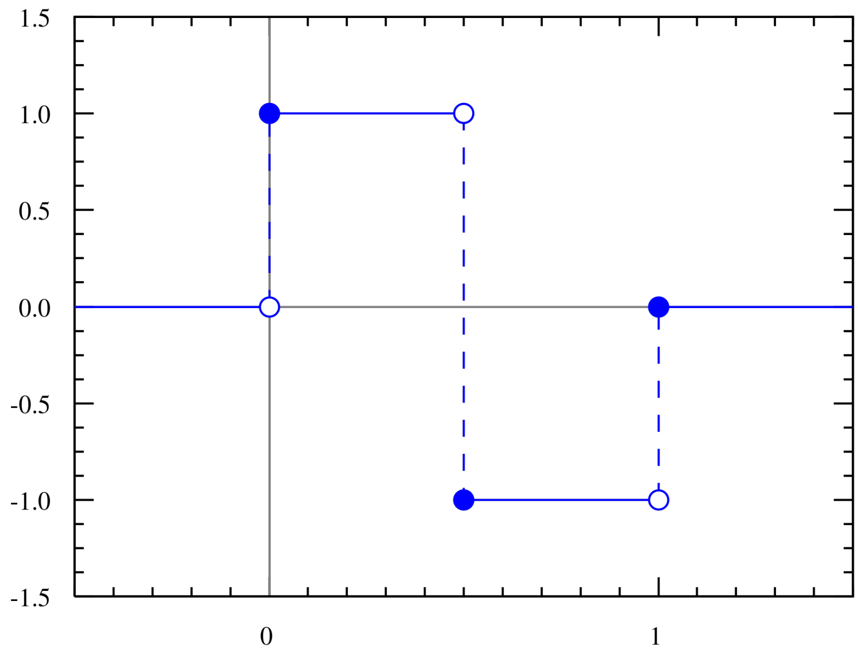

Figure 2.1: The Haar mother wavelet.

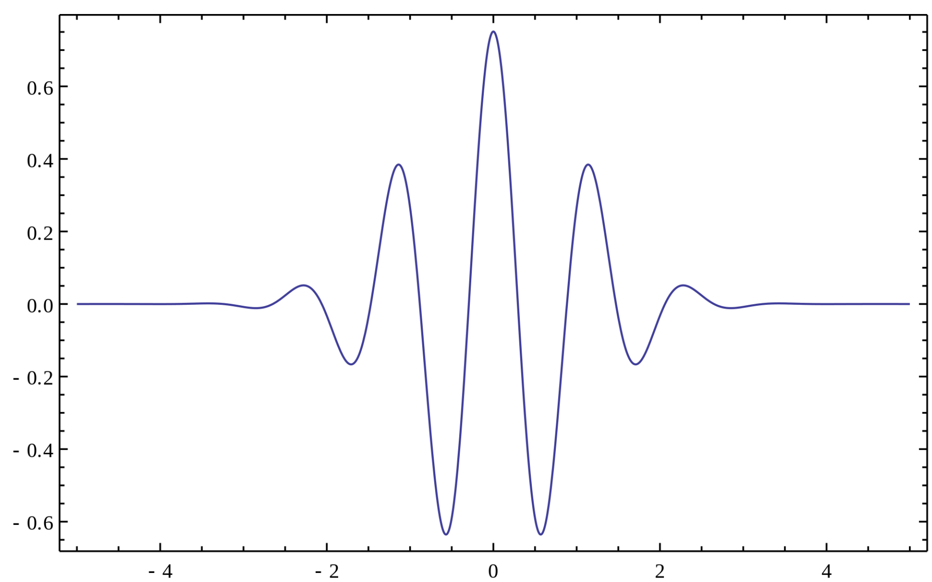

Figure 2.2: A Morlet Wavelet.

Chapter 3

Data Analysis

3.1 Preliminary Work

This section is not essential to the narrative and can be skipped. It is me doing a practice problem before going out to the "real world." I tried the fitting methods on a set of data that I generated following Dr. Lepage's article [4]. The data are not exactly similar to the ones I will be fitting later, because their error are small, and so the problem that this research tries to solve is not present here. It is generated from the lattice calculation of a correlation function of a simple harmonic oscillator. For the function and the value of some constants, refer to the paper. I show the data of one run of my Python code in Table 3.1.

Here are some of my fitting attempts: Fig. 3.1 is a fit to the data using Fourier series. The fit is terrible, as you can see directly from the plot, or from the chi2/dof measure which is on the scale of 10^2.

Fig. 3.2 is a fit using Morlet wavelets. This fit has chi2/dof = 5, and I had to make the prior uncertainties large to include all the parameter values, because they are quite far away from each other, unlike the parameters I got in the Lattice QCD data, which you will see later. This data is hard to fit well with a few parameters because its uncertainties are small. Even if the plot looks fine, the calculated values from the

t	$G(t)$
0	0.4803(56)
0.5	0.2921(37)
1	0.1808(33)
1.5	0.1132(30)
2	0.0713(29)
2.5	0.0445(28)
3	0.0276(27)
3.5	0.0164(27)
4	0.0099(27)
4.5	0.0050(27)
5	0.0012(28)
5.5	-0.0021(29)
6	-0.0030(30)
6.5	-0.0057(31)
7	-0.0093(33)
7.5	-0.0117(37)
8	-0.0146(57)

Table 3.1: Data from S.H.O.

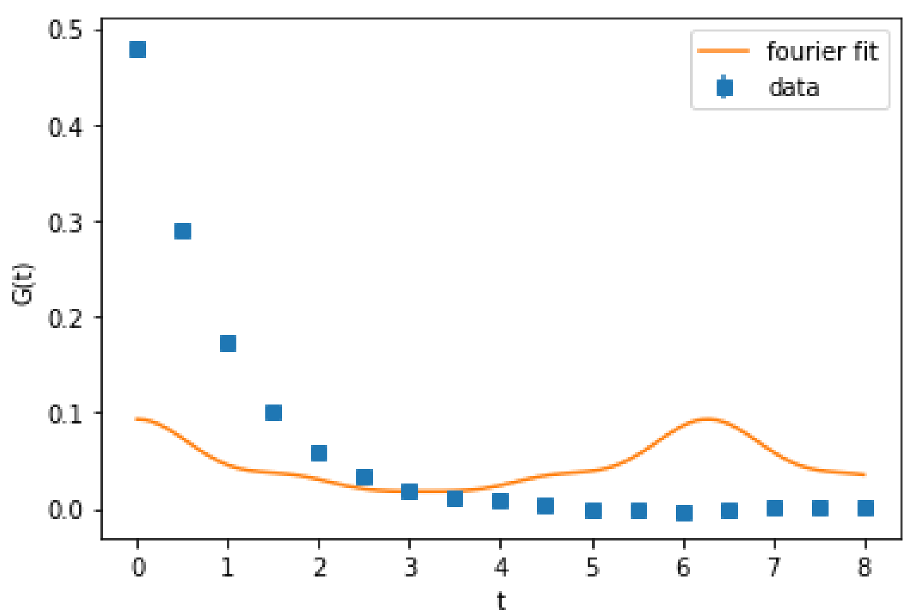

Figure 3.1: Fit to data from Table 3.1 using the Fourier series. The uncertainties of the data are smaller than the plotting symbol, so we do not see them.

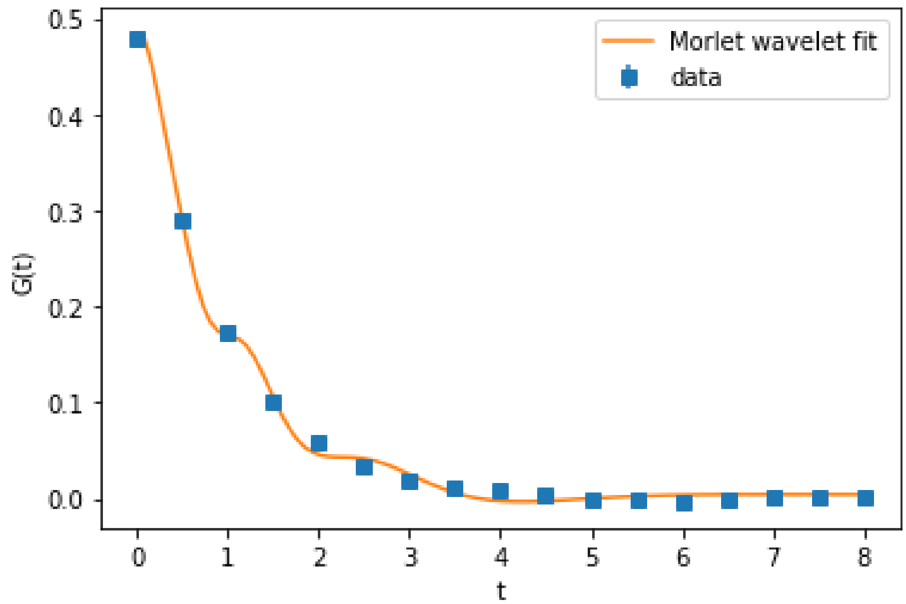

Figure 3.2: Fit to data from Table 3.1 using Morlet Wavelets. Uncertainties of data are smaller than the plotting symbol.

model are not close enough to the data points compared to their uncertainties.

3.2 Lattice QCD Data

Now we are applying the theories to the analysis of some lattice QCD data. These data are computer-generated in a mid-step of calculating a PDF. The quantity is a function of t or x; they should be the same thing. When we have some time series like this, we do a Fourier transform of them to get from the position to the momentum plane, which is the variable we want for PDF. Table 3.2 is a table of their values.

3.2.1 Analytical Fit

Theoretically, these data should go like, in approximation at large t's [5]:

$$f(x) = A + B\,t\,e^{-ct}. \tag{3.1}$$

t	G(t)
2	0.000575(51)
3	0.000672(65)
4	0.000745(79)
5	0.000920(96)
6	0.000442(36)
7	0.00089(11)
8	0.00105(14)
9	0.00100(14)
10	0.00127(20)
11	0.00124(26)
12	0.00109(32)
13	0.00119(43)
14	0.00166(63)

Table 3.2: Lattice QCD Data.

Least Square Fit:
chi2/dof [dof] = 0.27 [12]   Q = 1   logGBF = 73.155
Parameters:

A	0.00129 (19)	[0.30 (40)]
B	-0.00077 (14)	[0.30 (60)]
C	0.397 (86)	[0.30 (30)]

Table 3.3: Properties Table Using the Analytical Function.
Entries of the second column are the returned parameters of the fit. Entries of the third column are the priors (the a priori guess of the parameters) that I put in.

The first thing I did was to use this analytical function to fit the data. It should fit to large t's better, since at small t's some other nonessential functions are in the mix, but when t is large, these functions disappear. I show a figure of the analytical function fit to the data is shown in Fig. 3.3. The fit function goes through the dots at small t but is further away from the means at large t's. This is expected because lsqfit program (program: [6]) tries to find the best fit through reducing the quantity chi2/dof to its minimum. chi2 is calculated using:

$$\chi^2 = \sum_i \frac{(O_i - C_i)^2}{\sigma^2} \tag{3.2}$$

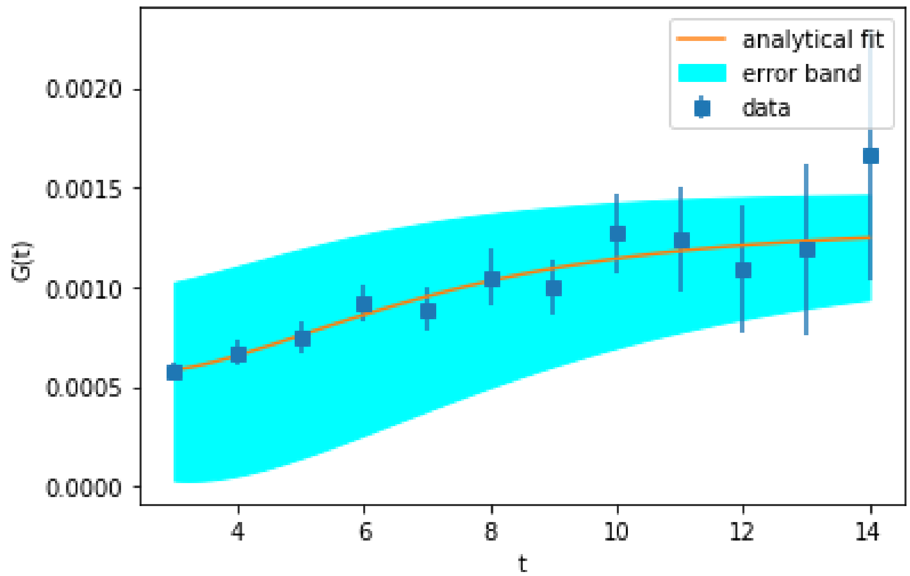

Figure 3.3: Analytical Function Fit

fitted to the whole range, chi2/dof = 0.27.

where O_i is the observed value, C_i the calculated value, and σ is the standard deviation of O_i, and then this value is divided by the number of data points (= dof). To minimize this, the fit function would want to have its C_i's near the E_i's. And because in the large t region, the data have larger error bars, C_i could be farther to E_i than in the small t region since their difference is going to be divided by the uncertainties. The fit prioritizes being closer to the small t's. The line conforms well to the data in Fig. 3.3. Table 3.3 gives the fit properties. The quantities Q gives "the probability that the chi**2 from the fit could have been larger, by chance, assuming the best-fit model is correct. Good fits have Q values larger than 0.1 or so. Also called the p-value of the fit [6]." LogGBF is the likelihood that this set of data comes from the model that I put in. It looks to be an excellent fit.

When I did this fit, I got two sets of parameters that both gave a good fit. It is normal. The difference is that the other set of parameters has $B > 0$, and the shape of the function has a maximum and then tapers off to 0. In the parameters that I

Least Square Fit:		
chi2/dof [dof] = 2.3 [9]	Q = 0.015	logGBF = 52.717
Parameters:		
constant	0.000826 (37)	[0.00 (30)]
$C_{2,0}$	0.00048 (12)	[0.00000 (50)]

Table 3.4: Least Square Fit Results Using Haar Wavelets.

have used, $B < 0$, and the function has a minimum before rising up and levelling off to 0 (assuming $A = 0$). I did not include the other set, because I looked at my professor's paper and they all have $B < 0$ and he says that the data would rise to and remain at a constant (rather than going up a peak and falling off to a constant).

[I have to add a disclaimer about the error band: the way it is produced is wrong, but I was told it gives an estimate of the real error band. To get the right error band, we need to take many steps back to the jackknife step in data generation, but the data of that is not available to me.]

The quantity that we are trying to get for the next step of calculating PDF is A, the constant term. This is the level that the data will stay at when t is large, as the t component of the analytical fit function goes to 0 in the limit of t = infinity.

3.2.2 Haar Wavelets Fit

Then I went on to try fitting the data using the Haar wavelet family. The result is in Fig. 3.4 and the corresponding fit properties are given in Table 3.4. The fit is not very good. I tried using different wavelet terms by changing j and k and the range. The results are similar. The best chi2/dof is around 2, sometimes 1.9. It is understandable because Haar wavelets are step functions, so they do not conform well to data that might require more fluidity from the fit function.

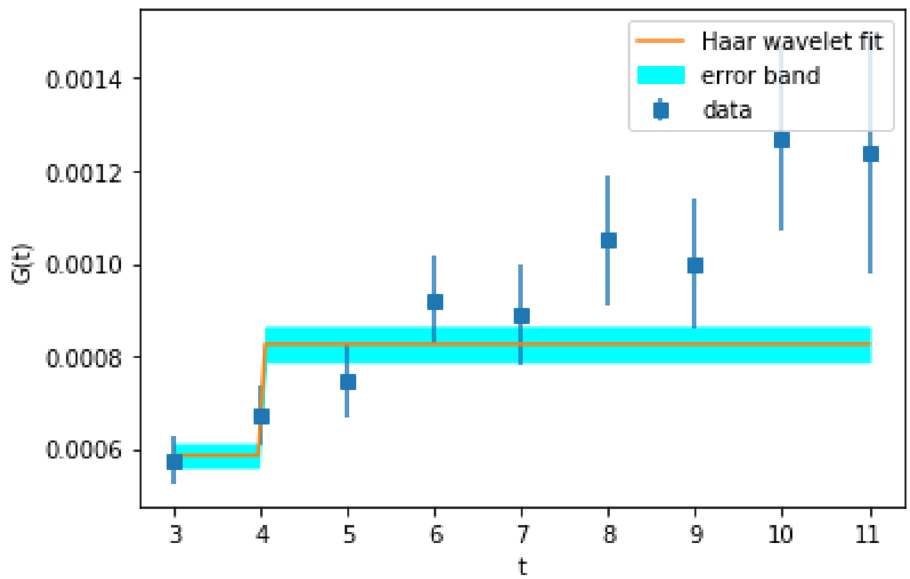

Figure 3.4: Haar wavelet fit result.

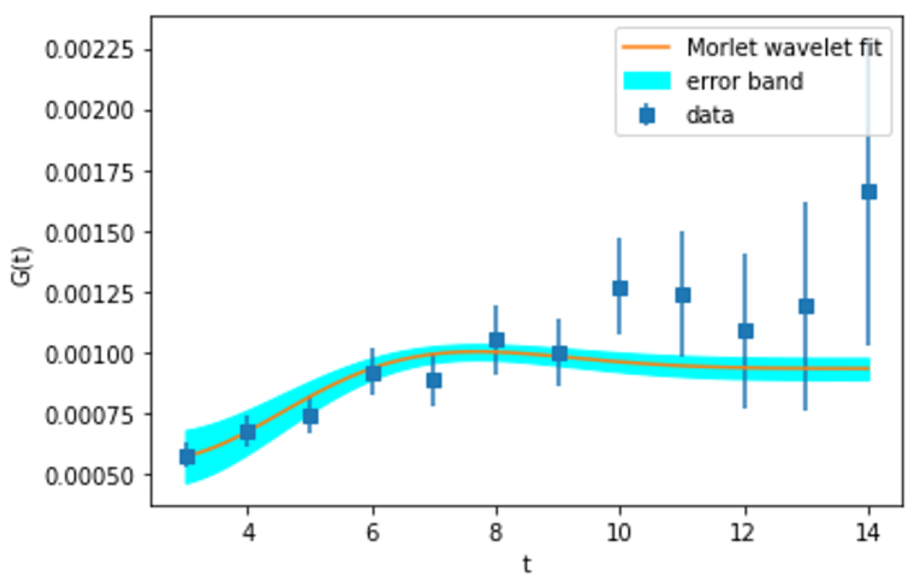

Figure 3.5: Morlet Wavelet Fit 1.

Least Square Fit:

chi2/dof [dof] = 0.7 [12]   Q = 0.75   logGBF = 81.536

Parameters:		
constant	0.000934 (44)	[0.000 (20)]
$C_{-1,-1}$	-0.00142 (25)	[0.0000 (14)]

Table 3.5: Morlet Wavelet Fit 1 Properties.

fitted to the whole range.

Least Square Fit:

chi2/dof [dof] = 0.41 [12]   Q = 0.96   logGBF = 79.772

Parameters: constant	0.00091 (11)	[0.00 (20)]
2,1	0.00050 (29)	[0.00000 (66)]
2,2	0.00027 (37)	[0.00000 (66)]
3,1	0.00066 (51)	[0.00000 (66)] *
3,2	-0.00035 (61)	[0.00000 (66)]

Table 3.6: Morlet Wavelet Fit 2 Properties.

fitted to the whole range.

3.2.3 Morlet Wavelets Fit

The method we have more hope for is Morlet wavelets because they are continuous. The fit that I get is in Fig. 3.5, and the properties table in Table 3.5. I used $\sigma = 2$. There is no real reason other than I tried 1 and 3 and found 2 is better than both of them, so I thought maybe that is the value to use. I added more wavelet terms, but the fit does not get better than this. So it already fits the data well. It is much better than Haar wavelets, and compared to the analytical function, it extracts A from the data to better precision; the first digit of the error starts at 5 digits after the point. Then I used more terms from the basis and changed which terms to put into the fit function. Fig. 3.6 gives a good fit. Table 3.6 gives its properties. You can see in the first column that m, n, labels for the terms, have changed. Chi2 is closer to 1 than Fit 1, which means it is better; logGBF is a little worse but is not a big difference.

Then I changed the range of fitting. I show a plot in Fig. 3.7 and the properties

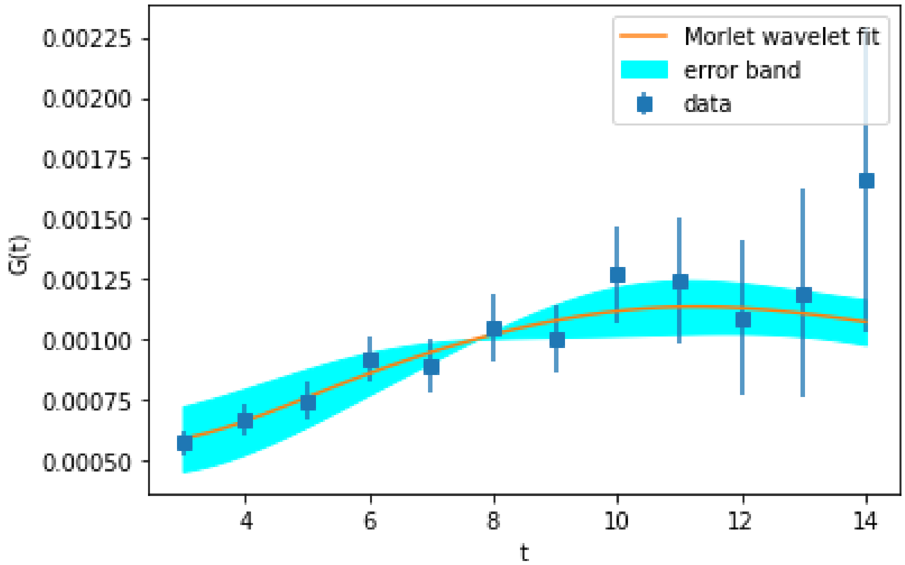

Figure 3.6: Morlet Wavelet Fit 2.

Least Square Fit:
chi2/dof [dof] = 0.95 [9]   Q = 0.48   logGBF = 60.636

Parameters:

constant	0.000953 (47)	[0.000 (20)]
$0, 0$	0.0105 (47)	[0.0100 (47)]
$1, -1$	0.0125 (24)	[0.0100 (47)]
$1, 0$	0.0044 (12)	[0.0100 (47)]

Table 3.7: Fit 3 Properties

table Table 3.6. The chi2/dof and logGBF measures are worse. From my experience, this range is harder to fit than from $t = 3$ to 14. But the shape of the function is similar to the first one. They are both produced out of the same data from one system, so I would expect them to have the same shape.

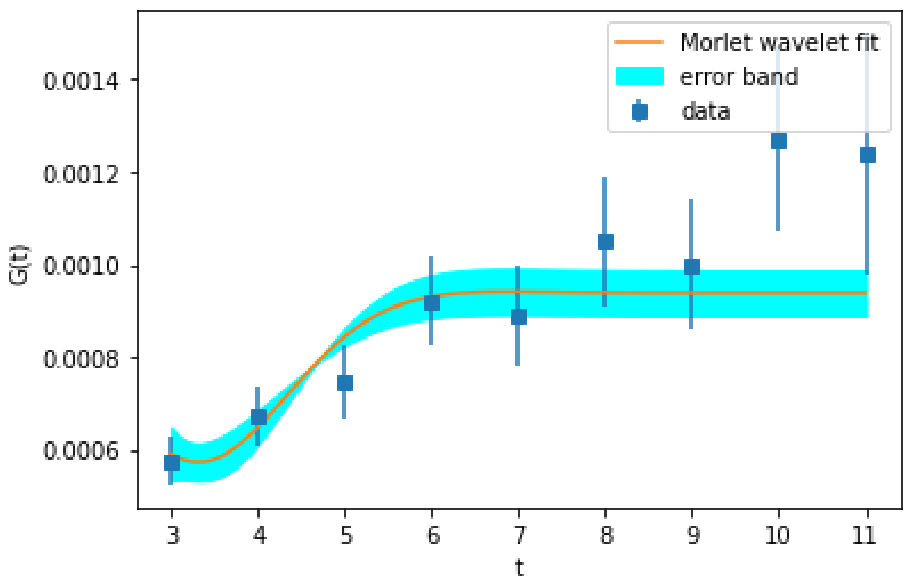

Figure 3.7: Morlet Wavelet Fit 3.
fitted to range [3:11]

Chapter 4

Results and Conclusions

4.1 Results

Because me and my professors have different views on this, I am going to write both down so I can have an account to myself and notes of my professors' views, and to pass the thesis course.

My view is that unless wavelets reconstruct the second term, $B\,t\,e^{-ct}$, in the analytical function, there is no justification that the asymptote from the wavelet fit is the same thing as the asymptote of the data, or that of the analytical function. To ask my advisor to consider this view, I made plots showing how they go into different directions after this range in fig. 4.1 and fig. 4.2. I have no reason to expect their asymptotes to be the same line.

[Another way to consider this is that a wavelet fit *always* has an asymptote, whether the data has it or not. Suppose you fit a line with wavelets. Outside the range you are fitting, the line might go on, or you might say it is zero outside the range, but the wavelet fit would stay at some level. You could say, no, let's think about it as an offset rather than asymptote, but still, these two offsets are not the same thing.

Since I had this thought, I was focused on reconstructing the analytical expression. But I have crossed it out because we have discrete data.]

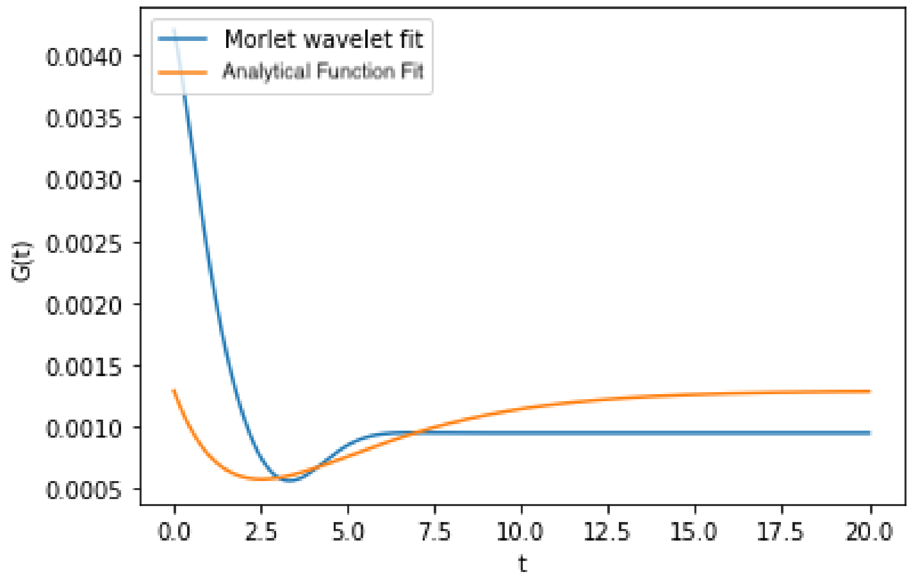

Figure 4.1: Morlet Wavelet Fit 1 and Analytical Function Fit on the same picture, on a bigger range than the range of the data.

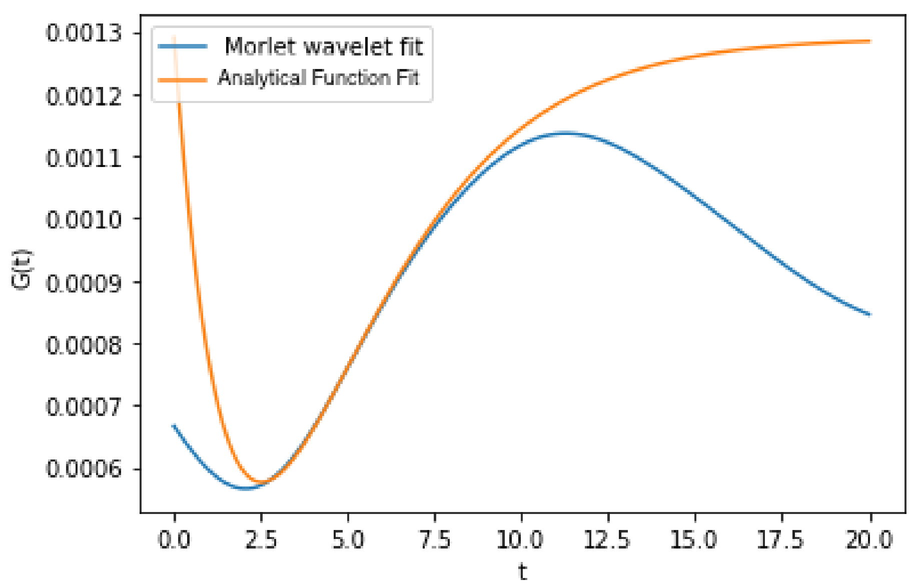

Figure 4.2: Morlet Wavelet Fit 2 and Analytical Function Fit on the same picture, on a bigger range than the range of the data.

I think the idea of what I have been doing is wrong. Since we have discrete data points, we do not reconstruct the function, and the data does not go like wavelets. A basis which does not model the quantity cannot get information beyond the data points we have already known, less on the quantity they represent from the system. It does not grasp anything in the data itself, and whatever it gives out is not from the data (it comes after the data in time, but not from the data). That is why the fit function goes crazy where it does not have them. It merely draws a curve across the data points, and I can do that too by hand and give all kinds of constant values. Even if we were fitting a continuous signal, thinking of this with Fourier series, what would be the point of fitting a Fourier series to data of a non-periodic function? Would it give us the frequency signal apart from noise? (I am not sure about the answer to the second question. I don't know much about data analysis. All I learned in physics class is that a basis reconstructs a function, but I haven't got to know how they can extract information from noisy data. So it could also be that there is something going on that I don't understand.) Because I do not agree with my professors on this point at present, I do not share their idea and plan for the project. Rather than telling us a posteriori if wavelets fit the data well, these plots, to me, manifest the lack of any solid reasoning at the start.

My views end here. The part from here starts my professors' view. My advisor and Prof. Armstrong think fitting data with a sum of wavelets in this range can give us the asymptote of the data. They say it is ok if we do not have a physical interpretation of the wavelet fit. It gives an estimate of the quantity that we want.

4.2 Plans for Future Work

My professors' suggestion is to test wavelet fitting on more data sets to see if they give us the correct asymptotic value. They suggested that we make fake data whose expression we decide, so we know the constant, and then fit it with wavelets to compare the result to the constant we put in. We can choose the number of data points we make, which will allow us to add in more wavelet terms. We will add another small-valued function to the true form to make it similar to our situation. As we know, in our system, there are some other functions when t is small. We will also add noise into it. With all these disruptions, we see if wavelets can approximately go with the true form and not be affected by the small-valued function and noise. The plan is to see whether wavelets are generally useful other than on this data set.

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