A Spectral Fit to Riemann's xi function

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1 Introduction

Originally proposed in 1859, the Riemann Hypothesis is regarded by many as the most important unsolved problem in Pure Mathematics, with a substantial prize for proving it. The usual formulation of this problem is that all of the (non trivial) zeros of the Zeta function have real part equal to 1/2. However, the xi function , a related function, provides a nicer way to phrase the Hypothesis, which is actually the way Riemann Originally stated it.

Definition 1.1 (Riemann xi Function)**.** Suppose $\omega \in \mathbb{C}$. Then the xi function of ω, denoted $\xi(\omega)$ is

$$\xi(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}\Phi(t)dt$$

where

$$\Phi(t) = \Sigma_{n\geq 1}(4\pi^2 n^4 e^{9t/2} - 6\pi n^2 e^{5t/2})e^{-\pi n^2 e^{2t}}.$$

In terms of the original zeta function, this can be written as:

$$\xi(\omega) = \frac{1}{2}s(s-1)\pi^{-s/2}\Gamma(\frac{s}{2})\zeta(s).$$

where $s = i\omega + 1/2$.

The Riemann Hypothesis states that all of the zeros of this function are real. This means that if the zeros of the xi function are also eigenvalues of a self adjoint linear operator, then this proves the Riemann Hypothesis. The general idea of relating the non trivial zeros of the Zeta function to a self adjoint operator is known as the Hilbert-Polya conjecture, which is also explored in various papers. This has led to an interest in the problem from a perspective relating to quantum mechanics, in particular looking at Schrodinger Operators, which are obtained from the time independent Schrodinger Equation $(-\partial_{xx} + V)\psi = E\psi$. In this project, I made an attempt to fit the zeros of the Riemann xi function to Spectra of Dirac and Schrodinger Operators, as well as the use of a Simulated Annealing method to try and improve the fit given by the latter case.

In order to get a "shooting function" to measure the eigenvalues of our operators, we will solve the differential equations (as the solutions we find will have the sufficient regularity) and evaluate the solutions at $x = 0$ as we need Dirichlet boundary conditions. We note that matching the zeros is what we are interested in, not matching the functions as a whole.

2 Dirac case

The first class of operators I have looked at are Dirac Operators. The reason for looking at these first is because $\frac{\omega}{2}$ will be used as an eigenvalue instead of $\frac{\omega^2}{4}$ (the latter has $\pm$ symmetry) and they have a relation to Schrodinger operators but haven't been previously explored compared to xi. The particular operator we will look at is the following differential one:

$$T : L^2(\mathbb{R}) \to L^2(\mathbb{R})$$
$$T(\psi_1, \psi_2) = ((-\partial_x + V(x))\psi_2, (\partial_x + V(x))\psi_1)$$

and the following equation to solve:

$$T(\psi_1, \psi_2) = \sqrt{E}(\psi_1, \psi_2).$$

Remark 2.1. *We are considering L^2 with boundary conditions of $\psi_1(0) = 0$ here.*

So that we can obtain the correct density of zeros of the shooting function, we will take $V(x)$ to be perturbations of $2\pi e^x$ by setting $V(x) = 2\pi n$ on $[\log(n), \log(n + 1))$ for $n \in \mathbb{N}$. This is an example of an unbounded self adjoint operator. Since the operator is self adjoint, the eigenvalues are all real. This makes it a contender for our fitting to the xi Function. It will be instead made piecewise constant by evaluating at $x = \log(n)\ \forall\ n \in \mathbb{N}$. If we combine this coupled pair of differential equations into 1 equation, this converts into a second order differential equation:

$$-\partial_{xx}\psi_1 + 4\pi^2 n^2 \psi_1 = E\psi_1$$

which has the solution on $x \in [\log(n), \log(n + 1))$

$$\psi_1(x, w) = A_n e^{k_n x} + B_n e^{-k_n x}$$

where $k_n(w) = \sqrt{4\pi^2 n^2 - E}$.

We then solved this and some graphs of our shooting function compared to the xi function (suitably scaled, exact scales given in full paper) are shown in this document.

3 Schrodinger Case and Simulated Annealing

Now what happens if we make the potential and time steps able to be modified to fit closer to the shooting function? We initially find the shooting function for

Figure 1: Dirac Shooting Function against xi Function for $\omega \in [0, 30]$

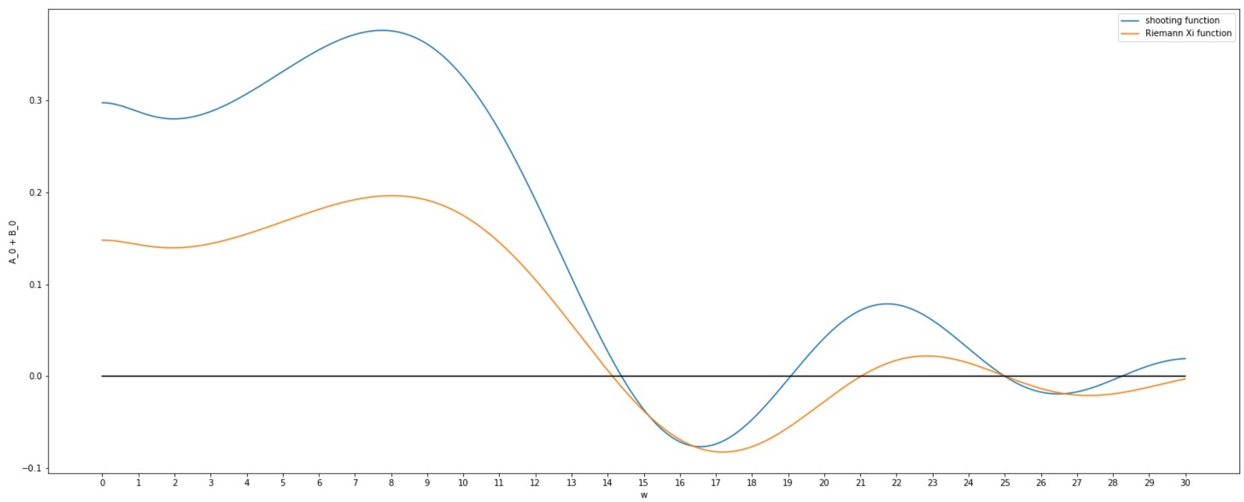


Figure 2: Dirac Shooting Function against xi Function for $\omega \in [30, 60]$.

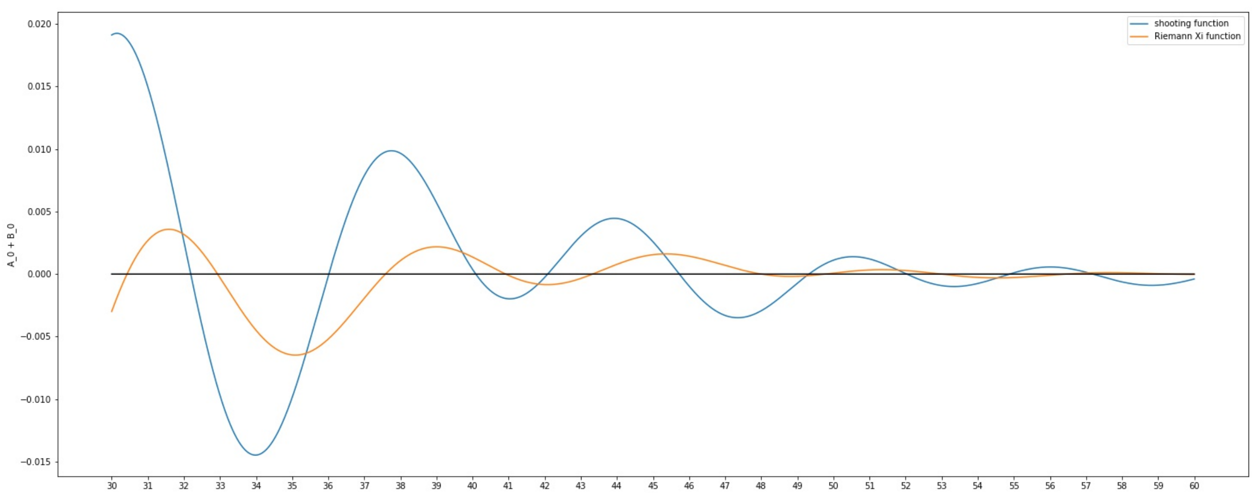
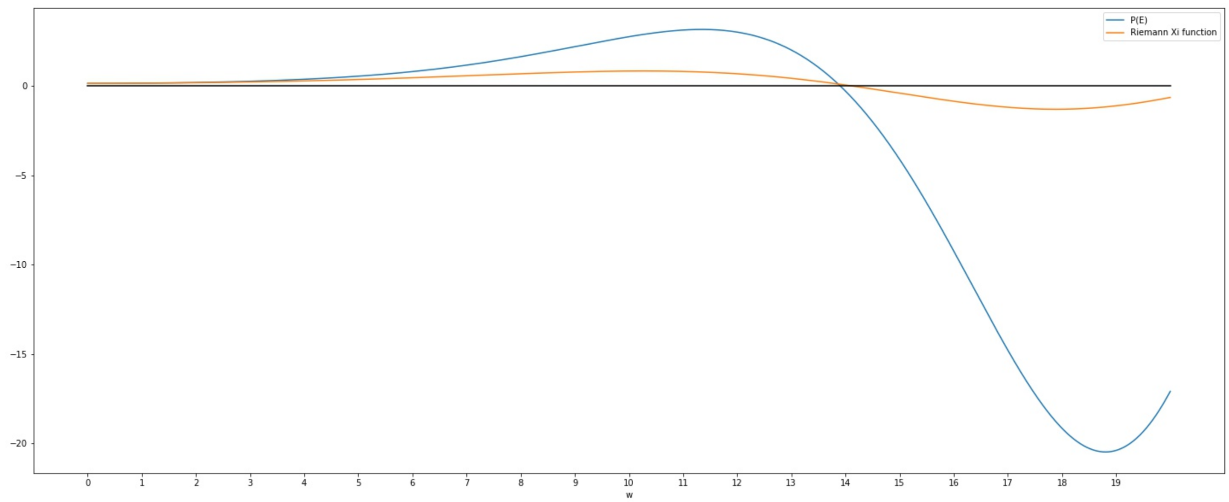


Figure 3: Schrodinger Shooting function against xi Function for $\omega \in [0, 20]$ with sum of squares on the real line, with improved potential.

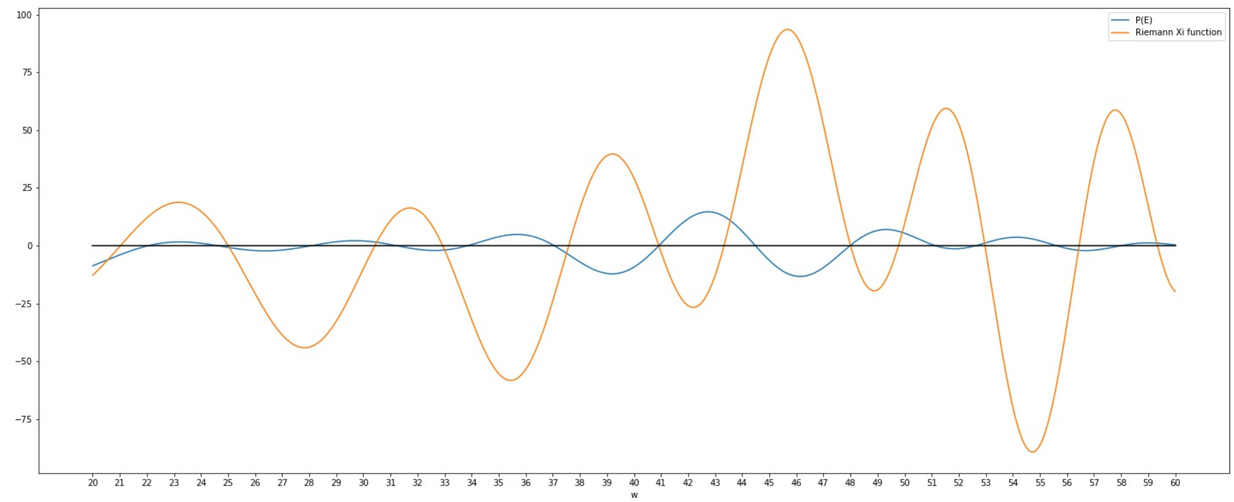


the Schrodinger case with $V(x) = 4\pi^2 e^{2x}$. This didn't fit closely enough so we ran simulated annealing to vary the time steps x_n and potentials V_n at each time step. Our minimiser was a sum of squares of the functions compared at points near the zeros on the real line and also points on the unit semicircle. The real line case is shown in (suitably scaled) graphs here with the potential changed to a better fitting $V(x) = 4\pi^2 e^{2x} - 9\pi e^x$.

4 Conclusion

From this project, we can see that although we have matched zeros closer to that of xi through the use of simulated annealing, we are still far off a very close fit. One method that could potentially be tried is the use of delta distributions in the potential rather than using just continuous or piece wise constant potentials. This could alleviate the issues of regularities of oscillations. In one of Remlings books, the setting proposed for general spectral problems is "canonical systems" of the form $Ju' = EH(x)u$, where $x \in \mathbb{R}^+$, $u \in L^2(\mathbb{R}^+, \mathbb{C}^2)$, $J = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$, H is a symmetric positive semi definite matrix and the boundary condition $u_2(0) = 0$ is imposed. We can transform the Schrodinger equation case into a system like this with $H = \begin{bmatrix} p^2 & pq \\ pq & q^2 \end{bmatrix}$ for functions p, q of x which are solutions of the

Figure 4: Schrodinger Shooting function against xi Function for $\omega \in [20, 60]$ with sum of squares on the real line, with improved potential



Schrodinger equation for $E = 0$ with basis boundary conditions at $x = 0$. If we look at problems of this form, but with p, q allowed to have discontinuities, we could potentially have some interesting results.